Conformational Preferences of β– and γ–Aminated Proline Analogues

Alejandra Flores-Ortega,[1] Jordi Casanovas[2,*]

Ruth Nussinov,[3,4] and Carlos Alemán,[1,*]

[1] *Departament d'Enginyeria Química, E. T. S. d'Enginyeria Industrial de Barcelona, Universitat Politècnica de Catalunya, Avda. Diagonal nº 647, 08028 Barcelona, Spain*

[2] *Departament de Química, Escola Politècnica Superior, Universitat de Lleida, c/Jaume II nº 69, 25001 Lleida, Spain*

[3] *Basic Research Program, SAIC-Frederick, Inc. Center for Cancer Research Nanobiology Program, NCI, Frederick, MD 21702, USA*

[4] *Department of Human Genetics Sackler, Medical School, Tel Aviv University, Tel Aviv 69978, Israel*

Table S1. Backbone dihedral angles (in degrees), pseudorotational parameters (A and P; in degrees) and relative energy (ΔE^{gp}; in kcal/mol) and free energy (ΔG^{gp}; in kcal/mol) of the minimum energy conformations characterized for Ac-L-Pro-NHMe at the B3LYP/6-31+G(d,p) level in the gas phase. These structural and energy parameters have been taken from *J. Org. Chem.* 2008, *73*, 3418

# Conf.	ω_0	φ	ψ	ω	(A, P)	ΔE^{gp}	ΔG^{gp}
t-γ_L[d]	-172.6	-83.4	70.3	-177.7	(37.4, -111.9)[a]	0.0[b]	0.0[c]
t-γ_L[u]	-173.9	-81.6	77.3	-175.9	(37.5, 75.8)[d]	1.0	1.3
t-α_L[u]	-171.0	-77.5	-11.5	175.9	(37.8, 89.2)[e]	4.9	4.0
c-α_L[d]	10.2	-90.9	-5.1	-179.6	(37.5, -111.5)[f]	3.3	2.3
c-α_L[u]	8.0	-79.2	-18.4	-177.1	(37.5, 90.1)[g]	4.2	3.6
c-ε_L[d]	1.2	-75.2	147.9	174.6	(36.8, -114.4)[h]	6.3	4.8
c-ε_L[u]	-0.1	-61.2	145.3	177.5	(37.4, 88.0)[i]	6.6	5.0

[a] χ^0= -13.9º, χ^1= 31.4º, χ^2= -37.6º, χ^3= 28.7º and χ^4= -9.3º. [b] E= -573.315217 a.u. [c] G= -573.132049 a.u. [d] χ^0= -10.3º, χ^1= -13.4º, χ^2= 31.0º, χ^3= -36.6º and χ^4= 29.8º. [e] χ^0= 0.5º, χ^1= -22.9º, χ^2= 36.1º, χ^3= -35.4º and χ^4= 22.0º. [f] χ^0= -13.8º, χ^1= 31.4º, χ^2= -37.6º, χ^3= 29.0º and χ^4= -9.5º. [g] χ^0= -0.1º, χ^1= -22.1º, χ^2= 35.7º, χ^3= -35.2º and χ^4= 22.3º. [h] χ^0= -15.2º, χ^1= 31.6º, χ^2= -36.7º, χ^3= 27.4º and χ^4= -7.5º. [i] χ^0= 1.3º, χ^1= -23.3º, χ^2= 36.0º, χ^3= -34.6º and χ^4= 21.2º.

Table S2. Atomic Coordinates (in Å), energies (in atomic units) and free energies (in atomic units) of the minimum energy conformations calculated for Ac-βtAmp-NHMe, Ac-βcAmp- NHMe, Ac-γtAmp- NHMe, Ac-γcAmp- NHMe.

Ac-βtAmp- NHMe

t-γ_L[d]

E= -628.6674459 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.517163
3	7	0	1.211249	0.000000	2.136426
4	6	0	2.526446	-0.046884	1.462935
5	1	0	2.662663	0.818353	0.806314
6	1	0	2.606843	-0.951357	0.845598
7	6	0	3.527966	-0.063959	2.629175
8	1	0	3.794359	0.957771	2.911871
9	1	0	4.438605	-0.617762	2.391015
10	6	0	2.754507	-0.714998	3.790048
11	7	0	2.832023	-2.177057	3.715109
12	1	0	3.164401	-0.400854	4.750957
13	6	0	1.332810	-0.131871	3.606150
14	1	0	0.559331	-0.823830	3.955881
15	6	0	1.141423	1.225711	4.330792
16	8	0	2.076682	1.814304	4.877199
17	7	0	-0.132950	1.682284	4.329309
18	1	0	-0.805298	1.178356	3.753998
19	6	0	-0.487282	2.964793	4.918059
20	1	0	-1.573168	3.016537	5.019606
21	1	0	-0.145066	3.805224	4.301739
22	1	0	-0.026345	3.060350	5.903975
23	8	0	-1.060242	0.007490	2.161896
24	1	0	-1.034624	-0.034097	-0.340275
25	1	0	0.543668	-0.860873	-0.403921
26	1	0	0.478096	0.904172	-0.392675
27	1	0	2.402675	-2.608826	4.528871
28	1	0	2.355599	-2.542621	2.893807

c-ε_L[u]

E= -628.6629998 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.471143
3	6	0	1.347674	0.000000	-0.550526
4	1	0	-0.100230	-1.023144	1.858974
5	1	0	-0.852488	0.576317	1.832880
6	6	0	1.364409	0.604694	1.810041
7	6	0	2.273782	0.037951	0.705108
8	1	0	1.528059	0.908361	-1.144740
9	6	0	1.692280	-1.219564	-1.436322
10	1	0	1.714644	0.345941	2.814204
11	1	0	1.322396	1.699180	1.732323
12	1	0	2.533239	-0.995184	0.967749
13	8	0	0.906328	-2.135719	-1.655773
14	6	0	-1.182929	0.118058	-0.688760
15	8	0	-2.258063	0.133554	-0.088441
16	6	0	-1.115043	0.239171	-2.198962
17	1	0	-2.077568	0.615125	-2.546560
18	1	0	-0.318950	0.912025	-2.535305
19	1	0	-0.928432	-0.746021	-2.635132
20	7	0	2.952737	-1.162568	-1.947988
21	1	0	3.580016	-0.472364	-1.543190

22	6	0	3.507008	-2.254353	-2.735812
23	1	0	4.355443	-1.881800	-3.314424
24	1	0	3.840640	-3.089945	-2.107617
25	1	0	2.742135	-2.629445	-3.418085
26	7	0	3.532110	0.720105	0.395438
27	1	0	3.389740	1.725067	0.309477
28	1	0	4.219421	0.574161	1.129957

c-α_L[u]

E= -628.6581046 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.478447
3	6	0	1.358642	0.000000	-0.565353
4	1	0	-0.205977	-1.006783	1.866801
5	1	0	-0.794121	0.656283	1.838022
6	6	0	1.415002	0.461859	1.821162
7	6	0	2.279204	-0.135943	0.689228
8	1	0	1.585517	0.943484	-1.076256
9	6	0	1.625206	-1.110483	-1.597152
10	1	0	1.745957	0.135635	2.812048
11	1	0	1.476062	1.557438	1.786012
12	1	0	2.419782	-1.205555	0.890691
13	8	0	2.390992	-0.931217	-2.537949
14	6	0	-1.152591	0.328999	-0.680348
15	8	0	-2.229355	0.415186	-0.090977
16	6	0	-1.036394	0.571343	-2.174690
17	1	0	-0.313238	1.361784	-2.402221
18	1	0	-0.708332	-0.327746	-2.705617
19	1	0	-2.019502	0.864526	-2.542192
20	7	0	0.999224	-2.297782	-1.356746
21	1	0	0.264477	-2.309002	-0.663151
22	6	0	1.146084	-3.436610	-2.251910
23	1	0	2.189581	-3.517062	-2.561673
24	1	0	0.853675	-4.346603	-1.723328
25	1	0	0.530078	-3.332412	-3.153696
26	7	0	3.596535	0.424885	0.451698
27	1	0	3.569297	1.436262	0.350902
28	1	0	4.243180	0.194360	1.199167

c-ε_L[d]

E= -628.6581099 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.521397
3	7	0	1.216974	0.000000	2.147700
4	6	0	1.293634	-0.060894	3.619394
5	1	0	0.707025	-0.905056	3.989935
6	1	0	0.860626	0.850051	4.050679
7	6	0	2.797664	-0.202527	3.899063
8	1	0	3.063885	-1.260641	3.952895
9	1	0	3.109045	0.290819	4.822578
10	6	0	3.479427	0.434908	2.675007
11	7	0	3.594897	1.881366	2.842482
12	1	0	4.488397	0.040329	2.519466
13	6	0	2.528601	-0.012884	1.509994
14	1	0	2.572392	0.718980	0.694239
15	6	0	2.928776	-1.404712	0.982956
16	8	0	2.649785	-2.441100	1.578896
17	7	0	3.668178	-1.399414	-0.162486
18	1	0	3.834005	-0.527424	-0.641770
19	6	0	4.193956	-2.632039	-0.737141

20	1	0	4.739346	-2.389063	-1.650789
21	1	0	3.382196	-3.326226	-0.974291
22	1	0	4.869796	-3.128944	-0.034754
23	8	0	-1.046251	0.010775	2.169153
24	1	0	-1.037326	-0.012544	-0.334088
25	1	0	0.516345	-0.878283	-0.401516
26	1	0	0.490905	0.893861	-0.402263
27	1	0	4.032509	2.326081	2.040502
28	1	0	2.688416	2.319047	2.986971

Ac-βcAmp- NHMe

t-γ_L [d]
E = -628.6688963 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.481052
3	6	0	1.365148	0.000000	-0.559472
4	1	0	-0.605969	-0.823903	1.871604
5	1	0	-0.424117	0.940422	1.855526
6	6	0	1.483258	-0.128857	1.850508
7	6	0	2.220522	0.487794	0.648918
8	1	0	1.398320	0.706859	-1.394850
9	6	0	1.739137	-1.406383	-1.088034
10	1	0	1.770471	-1.180257	1.943522
11	1	0	1.727236	0.381114	2.785418
12	1	0	2.088607	1.577388	0.690207
13	8	0	2.463055	-2.186396	-0.459443
14	6	0	-1.092340	0.151183	-0.797452
15	8	0	-0.994655	0.182368	-2.034021
16	6	0	-2.437710	0.275102	-0.108268
17	1	0	-3.204723	0.381427	-0.874891
18	1	0	-2.654374	-0.609995	0.499687
19	1	0	-2.467312	1.145652	0.556078
20	7	0	1.205013	-1.698499	-2.297245
21	1	0	0.478367	-1.070366	-2.636133
22	6	0	1.366996	-3.009477	-2.908430
23	1	0	0.727112	-3.764239	-2.434460
24	1	0	1.110852	-2.938870	-3.967541
25	1	0	2.404502	-3.334072	-2.807026
26	7	0	3.646861	0.223936	0.660729
27	1	0	4.139036	0.786923	-0.026259
28	1	0	3.818759	-0.758526	0.459623

t-α_L[d]
E = -628.6624383 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.519675
3	7	0	1.229839	0.000000	2.138049
4	6	0	2.523623	-0.197481	1.444021
5	1	0	2.743656	0.638878	0.772116
6	1	0	2.499307	-1.114422	0.840903
7	6	0	3.533711	-0.324046	2.587758
8	1	0	3.899554	0.663637	2.894460
9	1	0	4.399462	-0.934529	2.320979
10	6	0	2.717316	-0.946660	3.729945
11	1	0	2.523484	-1.997463	3.479443
12	7	0	3.418475	-0.932653	4.996829
13	6	0	1.331535	-0.209963	3.590338
14	1	0	0.506446	-0.841423	3.929311
15	6	0	1.242668	1.067309	4.438894

16	8	0	1.222910	0.983946	5.667642
17	7	0	1.240065	2.252911	3.774123
18	1	0	1.094934	2.211692	2.775543
19	6	0	1.027871	3.516892	4.465241
20	1	0	1.423981	4.332465	3.855589
21	1	0	1.553546	3.489948	5.420834
22	1	0	-0.035528	3.698113	4.663368
23	8	0	-1.043977	0.013756	2.169480
24	1	0	-1.030789	0.103651	-0.337979
25	1	0	0.411104	-0.937148	-0.392336
26	1	0	0.601700	0.818156	-0.410331
27	1	0	3.501321	0.014837	5.357517
28	1	0	2.893744	-1.444964	5.700705

c-α_L[d]
E = -628.6619761 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.518934
3	7	0	1.221102	0.000000	2.155732
4	6	0	1.265130	0.209889	3.618891
5	1	0	0.723961	-0.586711	4.135726
6	1	0	0.763202	1.152656	3.868956
7	6	0	2.762424	0.239855	3.925802
8	1	0	3.160283	-0.768778	4.081941
9	1	0	2.993272	0.833800	4.815161
10	6	0	3.397001	0.820014	2.649662
11	1	0	3.209149	1.906844	2.631509
12	7	0	4.810943	0.485403	2.528283
13	6	0	2.520404	0.217016	1.505556
14	1	0	2.439667	0.937528	0.686652
15	6	0	3.162971	-1.028603	0.865940
16	8	0	4.062212	-0.877533	0.036967
17	7	0	2.684646	-2.232896	1.259700
18	1	0	1.930330	-2.233687	1.932228
19	6	0	3.230780	-3.496102	0.787887
20	1	0	2.421575	-4.180886	0.518076
21	1	0	3.859400	-3.967697	1.551861
22	1	0	3.843299	-3.293249	-0.091539
23	8	0	-1.044087	0.000741	2.168998
24	1	0	-1.013333	-0.220570	-0.335725
25	1	0	0.694975	-0.730585	-0.423664
26	1	0	0.284668	0.988131	-0.380614
27	1	0	5.131113	0.521754	1.563396
28	1	0	5.383128	1.109283	3.088463

c-ε_L[d]
E = -628.6608904 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.475168
3	6	0	1.335881	0.000000	-0.568909
4	1	0	-0.541256	-0.871758	1.852668
5	1	0	-0.519078	0.892660	1.842252
6	6	0	1.490458	-0.002734	1.841222
7	6	0	2.178734	0.598998	0.601695
8	1	0	1.396264	0.662660	-1.438846
9	6	0	1.791249	-1.413365	-1.023694
10	1	0	1.847282	-1.029779	1.989693
11	1	0	1.703699	0.563339	2.752830
12	1	0	1.994409	1.679151	0.580513
13	8	0	1.109750	-2.416774	-0.832222

14	6	0	-1.188148	-0.111539	-0.672948
15	8	0	-2.253968	-0.138637	-0.057421
16	6	0	-1.132669	-0.182499	-2.188665
17	1	0	-2.156796	-0.178355	-2.561643
18	1	0	-0.591643	0.667471	-2.619628
19	1	0	-0.635653	-1.103105	-2.510071
20	7	0	2.974231	-1.428208	-1.698334
21	1	0	3.569175	-0.614576	-1.582618
22	6	0	3.571947	-2.675449	-2.155746
23	1	0	4.337149	-2.449983	-2.901787
24	1	0	4.026577	-3.244517	-1.334727
25	1	0	2.799117	-3.299115	-2.608368
26	7	0	3.623764	0.412057	0.462148
27	1	0	4.129838	1.141365	0.954788
28	1	0	3.922270	-0.478211	0.854610

c-α_L[u]
E = -628.6598999 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.484005
3	6	0	1.360422	0.000000	-0.550230
4	1	0	-0.594101	-0.832976	1.871944
5	1	0	-0.470992	0.922287	1.840379
6	6	0	1.490029	-0.079028	1.846392
7	6	0	2.177732	0.591401	0.635810
8	1	0	1.445932	0.645902	-1.426686
9	6	0	1.852275	-1.397749	-0.993047
10	1	0	1.826674	-1.118854	1.939183
11	1	0	1.712341	0.431955	2.787927
12	1	0	1.907816	1.657462	0.664897
13	8	0	2.975259	-1.534408	-1.482406
14	6	0	-1.160340	0.292070	-0.676273
15	8	0	-2.226307	0.400618	-0.071509
16	6	0	-1.071839	0.468691	-2.183427
17	1	0	-2.087214	0.473188	-2.579880
18	1	0	-0.598910	1.426878	-2.428654
19	1	0	-0.492562	-0.322262	-2.669310
20	7	0	0.987567	-2.427065	-0.806681
21	1	0	0.078607	-2.204713	-0.425087
22	6	0	1.288929	-3.795646	-1.198946
23	1	0	1.057599	-4.484443	-0.380990
24	1	0	0.715407	-4.090843	-2.084950
25	1	0	2.352436	-3.854606	-1.433201
26	7	0	3.616100	0.505233	0.482644
27	1	0	4.099504	0.673151	1.358461
28	1	0	3.918347	-0.374627	0.074718

t-α_L [u]
E = -628.6551592 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.478535
3	6	0	1.379702	0.000000	-0.542791
4	1	0	-0.225393	-1.002599	1.867976
5	1	0	-0.752025	0.684755	1.873897
6	6	0	1.430237	0.428506	1.826901
7	6	0	2.279575	-0.217477	0.707490
8	1	0	1.588734	0.981138	-0.981725
9	6	0	1.685875	-1.002517	-1.664071
10	1	0	1.741464	0.104412	2.824504
11	1	0	1.511055	1.521529	1.779380

12	7	0	2.607473	-1.628212	0.908142
13	1	0	3.225622	0.309781	0.562627
14	8	0	2.690399	-0.843486	-2.349175
15	6	0	-1.029462	0.477986	-0.780414
16	8	0	-0.860563	0.723061	-1.973092
17	6	0	-2.385630	0.660973	-0.116590
18	1	0	-2.643541	-0.163778	0.554693
19	1	0	-2.403962	1.588323	0.468180
20	1	0	-3.134400	0.740950	-0.905003
21	7	0	0.840501	-2.059575	-1.798281
22	1	0	-0.063529	-1.982273	-1.356141
23	6	0	0.994761	-3.002428	-2.896889
24	1	0	2.046423	-3.281319	-2.981421
25	1	0	0.400056	-3.894785	-2.687725
26	1	0	0.675328	-2.569843	-3.852957
27	1	0	3.229218	-1.749331	1.701607
28	1	0	1.789225	-2.214105	1.048477

Ac-γtAmp- NHMe

t-γ_L [u]

E = -628.6675146 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.468473
3	6	0	1.388714	0.000000	-0.520753
4	1	0	0.003124	-1.028379	1.853417
5	1	0	-0.876045	0.516533	1.863513
6	6	0	1.313912	0.709973	1.830032
7	6	0	2.264036	0.211838	0.729030
8	1	0	1.470911	0.823467	-1.236657
9	6	0	1.731831	-1.328139	-1.250597
10	1	0	1.660960	0.386752	2.823409
11	1	0	2.708623	-0.746792	1.009887
12	1	0	3.079341	0.915738	0.537392
13	8	0	2.460634	-2.184843	-0.746253
14	6	0	-1.041614	0.336508	-0.808520
15	8	0	-0.890535	0.476610	-2.031957
16	6	0	-2.407346	0.524733	-0.172575
17	1	0	-2.675217	-0.306490	0.486818
18	1	0	-2.434908	1.448588	0.416228
19	1	0	-3.140588	0.601382	-0.975306
20	7	0	1.179704	-1.444918	-2.479797
21	1	0	0.471331	-0.756096	-2.728196
22	6	0	1.334846	-2.653407	-3.274007
23	1	0	0.745649	-3.486664	-2.871118
24	1	0	1.008185	-2.446948	-4.295301
25	1	0	2.384115	-2.957482	-3.284193
26	7	0	1.125506	2.162782	1.725297
27	1	0	0.557133	2.519235	2.489570
28	1	0	2.017279	2.649284	1.761161

c-α_L[d]

E = -628.663016 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.520130
3	7	0	1.220637	0.000000	2.155210
4	6	0	1.274747	0.198371	3.615390
5	1	0	0.801850	-0.630133	4.147960
6	1	0	0.727685	1.110268	3.888952

7	6	0	2.775146	0.338545	3.923022
8	1	0	3.203171	-0.661651	4.065977
9	7	0	2.993936	1.069582	5.163825
10	6	0	3.340420	0.932755	2.612816
11	1	0	3.129103	2.009050	2.580970
12	1	0	4.415797	0.789535	2.485492
13	6	0	2.529586	0.218670	1.512233
14	1	0	2.434903	0.849302	0.624513
15	6	0	3.249614	-1.061544	1.034358
16	8	0	4.316239	-0.963064	0.430041
17	7	0	2.645912	-2.241849	1.327984
18	1	0	1.767034	-2.199772	1.825593
19	6	0	3.199323	-3.533057	0.949345
20	1	0	2.508425	-4.078152	0.297550
21	1	0	3.407745	-4.143460	1.834502
22	1	0	4.131280	-3.353011	0.412102
23	8	0	-1.045228	-0.000160	2.168150
24	1	0	-1.005810	-0.254404	-0.334544
25	1	0	0.718592	-0.705817	-0.426510
26	1	0	0.247448	0.998598	-0.379398
27	1	0	3.974720	1.072049	5.427558
28	1	0	2.687959	2.036922	5.086552

$c-\varepsilon_L$[u]

E = -628.6580176 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.469583
3	6	0	1.354598	0.000000	-0.555487
4	1	0	-0.076105	-1.026644	1.853317
5	1	0	-0.857117	0.566874	1.837934
6	6	0	1.359418	0.636762	1.811204
7	6	0	2.260857	0.055348	0.707498
8	1	0	1.509997	0.894627	-1.176844
9	6	0	1.681098	-1.258245	-1.382913
10	1	0	1.707414	0.322132	2.799731
11	1	0	2.559238	-0.962433	0.977172
12	1	0	3.158028	0.657942	0.551011
13	8	0	1.238979	-2.363070	-1.087574
14	6	0	-1.179616	-0.010057	-0.699083
15	8	0	-2.263567	-0.022461	-0.116158
16	6	0	-1.095967	-0.002819	-2.215825
17	1	0	-0.360033	0.712405	-2.598033
18	1	0	-0.822230	-0.998876	-2.579476
19	1	0	-2.082391	0.252500	-2.603302
20	7	0	2.539063	-1.041505	-2.421273
21	1	0	2.835543	-0.094994	-2.611150
22	6	0	3.047036	-2.110586	-3.269280
23	1	0	4.140799	-2.150626	-3.233806
24	1	0	2.642185	-3.051524	-2.895312
25	1	0	2.727995	-1.973489	-4.308075
26	7	0	1.388978	2.104848	1.784000
27	1	0	0.874945	2.485395	2.574704
28	1	0	0.934051	2.460465	0.945145

Ac-γcAmp- NHMe.

t-γ_L[d]

E = -628.6696739 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.516416
3	7	0	1.210928	0.000000	2.136356
4	6	0	2.521158	-0.096034	1.463069
5	1	0	2.722287	0.782187	0.844086
6	1	0	2.549963	-0.989997	0.827361
7	6	0	3.561570	-0.190158	2.603298
8	1	0	4.334605	-0.911591	2.321787
9	6	0	2.725279	-0.734117	3.794753
10	1	0	2.669198	-1.827608	3.743716
11	1	0	3.156489	-0.450706	4.756484
12	6	0	1.315272	-0.158154	3.604223
13	1	0	0.531651	-0.850556	3.928390
14	6	0	1.095525	1.193554	4.331133
15	8	0	2.030375	1.844360	4.810851
16	7	0	-0.195731	1.584275	4.400048
17	1	0	-0.860317	1.063585	3.829407
18	6	0	-0.576973	2.867902	4.970265
19	1	0	-1.655724	2.870976	5.138359
20	1	0	-0.314631	3.701982	4.307939
21	1	0	-0.061490	3.016403	5.921601
22	8	0	-1.060954	0.000389	2.161287
23	1	0	-1.034487	0.031210	-0.340991
24	1	0	0.483538	-0.899890	-0.396293
25	1	0	0.540761	0.865110	-0.398080
26	7	0	4.231670	1.095738	2.815905
27	1	0	3.657140	1.699494	3.405588
28	1	0	5.102018	0.951429	3.320416

t-γ_L[u]

E = -628.6673143 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.464635
3	6	0	1.393588	0.000000	-0.518990
4	1	0	0.064870	-1.026181	1.855590
5	1	0	-0.902324	0.466586	1.863532
6	6	0	1.288916	0.784093	1.810388
7	6	0	2.261180	0.322392	0.710302
8	1	0	1.455476	0.768137	-1.296163
9	6	0	1.757333	-1.372384	-1.151755
10	1	0	1.072030	1.852761	1.683889
11	1	0	2.772072	-0.593120	1.026541
12	1	0	3.023362	1.073831	0.492873
13	8	0	2.463369	-2.196771	-0.569110
14	6	0	-1.057975	0.214006	-0.829029
15	8	0	-0.906530	0.313818	-2.056298
16	6	0	-2.438059	0.324327	-0.204955
17	1	0	-2.656516	-0.520701	0.455300
18	1	0	-2.533178	1.244295	0.382961
19	1	0	-3.168150	0.350646	-1.013698
20	7	0	1.243257	-1.567225	-2.388696
21	1	0	0.533314	-0.905567	-2.696557
22	6	0	1.414129	-2.827649	-3.095053
23	1	0	0.794336	-3.625193	-2.666558
24	1	0	1.137707	-2.684546	-4.141702
25	1	0	2.457966	-3.143706	-3.036376
26	7	0	1.847995	0.611950	3.141486

27	1	0	1.221021	0.938727	3.870536
28	1	0	2.085065	-0.359107	3.328591

c-α_L[d]

E = -628.6653972 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.516813
3	7	0	1.217981	0.000000	2.149583
4	6	0	1.264428	0.064848	3.615093
5	1	0	0.589354	-0.678461	4.048196
6	1	0	0.933901	1.050244	3.970218
7	6	0	2.736970	-0.182590	3.952677
8	1	0	3.017103	0.347613	4.873658
9	6	0	3.471861	0.414118	2.736100
10	1	0	3.595803	1.491086	2.887123
11	1	0	4.468476	-0.012256	2.586811
12	6	0	2.536532	0.173663	1.518928
13	1	0	2.544228	1.046305	0.859093
14	6	0	2.997017	-0.987777	0.605148
15	8	0	3.453838	-0.737502	-0.511911
16	7	0	2.870799	-2.239078	1.105061
17	1	0	2.684465	-2.322021	2.105534
18	6	0	3.341769	-3.400495	0.366233
19	1	0	2.899908	-4.300365	0.800213
20	1	0	4.435522	-3.489690	0.391206
21	1	0	3.038060	-3.317933	-0.679464
22	8	0	-1.043410	-0.015362	2.172336
23	1	0	-1.032775	0.097557	-0.334261
24	1	0	0.418027	-0.932621	-0.392194
25	1	0	0.597250	0.818683	-0.414160
26	7	0	2.984303	-1.635673	4.050271
27	1	0	2.435440	-2.037782	4.807094
28	1	0	3.962430	-1.817375	4.266699

c-α_L[u]

E = -628.6614753 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.471497
3	6	0	1.370687	0.000000	-0.553336
4	1	0	-0.119353	-1.018446	1.870370
5	1	0	-0.831206	0.599965	1.842042
6	6	0	1.384541	0.555704	1.833342
7	6	0	2.275926	-0.010839	0.704602
8	1	0	1.552763	0.902101	-1.146069
9	6	0	1.718988	-1.184992	-1.468567
10	1	0	1.348871	1.648991	1.745843
11	1	0	2.557901	-1.041217	0.956037
12	1	0	3.197352	0.553133	0.542483
13	8	0	2.707185	-1.122440	-2.197359
14	6	0	-1.128897	0.392779	-0.690764
15	8	0	-2.214230	0.503958	-0.124462
16	6	0	-0.971417	0.679415	-2.174876
17	1	0	-0.364382	1.578081	-2.334281
18	1	0	-0.488941	-0.141770	-2.712965
19	1	0	-1.965240	0.849483	-2.588326
20	7	0	0.917571	-2.277262	-1.358668
21	1	0	0.103410	-2.193984	-0.764874
22	6	0	1.135795	-3.502439	-2.112173
23	1	0	1.174954	-4.365630	-1.440022

24	1	0	0.340910	-3.662933	-2.849243
25	1	0	2.088806	-3.409882	-2.634496
26	7	0	1.750734	0.247606	3.208700
27	1	0	2.600181	0.729015	3.487776
28	1	0	1.898695	-0.750053	3.342682

t-α_L [u]

E = -628.6606213 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.468961
3	6	0	1.382391	0.000000	-0.535803
4	1	0	-0.065677	-1.025356	1.864337
5	1	0	-0.838249	0.572858	1.869906
6	6	0	1.373666	0.613325	1.830815
7	6	0	2.277999	0.052477	0.724426
8	1	0	1.515038	0.888042	-1.161422
9	6	0	1.772220	-1.187862	-1.426464
10	1	0	1.299294	1.702435	1.715460
11	1	0	2.602349	-0.958557	1.001874
12	1	0	3.176919	0.648436	0.563549
13	8	0	2.870429	-1.184323	-1.978364
14	6	0	-1.039241	0.397698	-0.809348
15	8	0	-0.869991	0.572018	-2.015364
16	6	0	-2.403465	0.586018	-0.163833
17	1	0	-2.429711	1.510045	0.425531
18	1	0	-3.140536	0.667053	-0.962861
19	1	0	-2.671643	-0.241697	0.500125
20	7	0	0.898572	-2.226677	-1.494546
21	1	0	-0.036864	-2.060693	-1.153238
22	6	0	1.125173	-3.357270	-2.383335
23	1	0	2.196052	-3.561141	-2.422425
24	1	0	0.601610	-4.235056	-1.996100
25	1	0	0.775980	-3.149549	-3.402203
26	7	0	1.897599	0.354710	3.162269
27	1	0	1.332369	0.781488	3.889986
28	1	0	1.972818	-0.640934	3.355256

c-ε_L[d]

E = -628.6601957 a.u.

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.519986
3	7	0	1.216816	0.000000	2.149571
4	6	0	1.286584	-0.023138	3.619668
5	1	0	0.619939	-0.793928	4.014200
6	1	0	0.955221	0.942273	4.026882
7	6	0	2.774371	-0.301602	3.927801
8	1	0	3.070807	0.214481	4.846818
9	6	0	3.482716	0.331871	2.712117
10	1	0	3.577919	1.412743	2.858729
11	1	0	4.480852	-0.086638	2.562772
12	6	0	2.528996	0.077752	1.512782
13	1	0	2.568084	0.921603	0.810888
14	6	0	2.910188	-1.210311	0.749640
15	8	0	2.558319	-2.330556	1.113849
16	7	0	3.697191	-1.014830	-0.341091
17	1	0	3.964780	-0.074770	-0.592268
18	6	0	4.242413	-2.130680	-1.105520
19	1	0	4.975825	-2.692815	-0.517926

20	1	0	4.723334	-1.739680	-2.003847
21	1	0	3.440634	-2.815074	-1.393553
22	8	0	-1.046660	-0.004916	2.167540
23	1	0	-1.033886	0.086085	-0.333970
24	1	0	0.423457	-0.931885	-0.388891
25	1	0	0.578837	0.834062	-0.412424
26	7	0	3.152084	-1.707774	4.075804
27	1	0	2.725385	-2.104956	4.908492
28	1	0	2.838231	-2.254740	3.273941

$c\text{-}\varepsilon_L$[u]

E = -628.6571276 a.u.

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.466598
3	6	0	1.353447	0.000000	-0.558033
4	1	0	-0.091028	-1.019864	1.862670
5	1	0	-0.842202	0.591461	1.831513
6	6	0	1.376670	0.579994	1.810031
7	6	0	2.259262	-0.012760	0.700633
8	1	0	1.521500	0.919216	-1.139602
9	6	0	1.658333	-1.226472	-1.441290
10	1	0	1.331142	1.675749	1.680567
11	1	0	2.504273	-1.044457	0.973862
12	1	0	3.191277	0.537076	0.537785
13	8	0	1.195057	-2.335091	-1.201518
14	6	0	-1.179802	0.041956	-0.695644
15	8	0	-2.262819	0.053411	-0.110395
16	6	0	-1.100143	0.072317	-2.212364
17	1	0	-0.336810	0.763184	-2.585411
18	1	0	-0.869957	-0.927943	-2.594093
19	1	0	-2.076427	0.375629	-2.590860
20	7	0	2.528857	-0.978424	-2.463279
21	1	0	2.813093	-0.024575	-2.633455
22	6	0	2.998333	-2.014275	-3.372410
23	1	0	2.552737	-1.905238	-4.367858
24	1	0	4.088297	-1.978467	-3.463138
25	1	0	2.701975	-2.979332	-2.960106
26	7	0	1.827734	0.179174	3.141280
27	1	0	1.182710	0.503643	3.857637
28	1	0	2.737163	0.580282	3.355510