High Level *ab initio* Calculations to Improve Protein Backbone Dihedral Parameters

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1 Equilibrium structures and total energies for GDA at various levels of theory

1.1 C7 conformer

GDA: C7 conformer, energy in hartrees.
RHF/6-31G(d)=-375.7479433

H	0.0000000000	0.0000000000	1.0000000000
C	1.0788683600	0.0000000000	1.0000000000
N	1.5450366188	0.9717655676	1.9717655676
C	1.5316894638	0.3111997163	-0.4253384127
H	1.4334514379	-0.9782496234	1.2962301675
C	2.7551334747	0.9046100303	2.5499501722
H	2.9263559472	1.6928301492	3.2814299979
O	3.5829741701	0.0703516943	2.3075018656
H	0.9587551043	1.7462729706	2.1852916548
N	2.8546644696	0.1844844769	-0.6408335968
H	3.2120875939	0.4193493646	-1.5391675891
H	3.4851253339	-0.0421480121	0.0965841477
O	0.7444499081	0.6329541937	-1.2711106547

GDA: C7 conformer, energy in hartrees.
RHF/6-31+G(d)=-375.7613763

H	0.0000000000	0.0000000000	1.0000000000
C	1.0787379800	0.0000000000	1.0000000000
N	1.5426191077	0.9723217103	1.9723217103
C	1.5326820702	0.3112585969	-0.4251356491
H	1.4328783099	-0.9790044745	1.2952965009
C	2.7481395067	0.9065649924	2.5605029061
H	2.9153124428	1.6908577009	3.2956320298
O	3.5806480525	0.0748190914	2.3170297367

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H          0.9469011193        1.7372290992        2.1979198841
N          2.8557556260        0.2046687310       -0.6450618049
H          3.2064236099        0.4189378594       -1.5520607316
H          3.4920588655       -0.0370501798        0.0834465476
O          0.7390846565        0.6189895108       -1.2738690724

GDA: C7 conformer, energy in hartrees.
MP2/6-311++G(d,p)=-377.0305112
H         -2.0588537704       -0.4730212882        0.2263094802
C         -0.9690621712       -0.4664420227        0.2248136681
N         -0.5069084151        0.5087470676        1.2041084105
C         -0.5060881330       -0.1105387810       -1.1917440401
H         -0.5938192898       -1.4506935120        0.5192372807
C          0.7441810216        0.4610906296        1.7284817251
H          0.9325598980        1.2576095937        2.4665953219
O          1.5842922963       -0.3810087685        1.4305496249
H         -1.1021420422        1.2876987412        1.4448026219
N          0.8054798580       -0.3968646727       -1.4336686390
H          1.2038252084       -0.0334430856       -2.2874758131
H          1.4165783936       -0.5898562048       -0.6491180627
O         -1.2720838966        0.3702425230       -2.0158917934

GDA: C7 conformer, energy in hartrees.
MP2/6-31G(d)=-376.8023289
H          0.0000000000        0.0000000000        1.0000000000
C          1.0904403600        0.0000000000        1.0000000000
N          1.5626752100        0.9751821559        1.9751821559
C          1.5541263924        0.3373283028       -0.4181362285
H          1.4565925343       -0.9856429274        1.3025912714
C          2.8073954749        0.9100960608        2.5053992220
H          3.0070899720        1.7008902249        3.2472791034
O          3.6450337591        0.0511526574        2.2134121055
H          0.9750189123        1.7672315863        2.2026307611
N          2.8726681424        0.0822268376       -0.6379015386
H          3.2717940353        0.4052028902       -1.5095795032
H          3.4834150907       -0.1282184576        0.1453580083
O          0.7820650772        0.7891337769       -1.2638284908

GDA: C7 conformer, energy in hartrees.
MP2/6-31+G(d)=-376.8329459
H          0.0000000000        0.0000000000        1.0000000000
C          1.0908129000        0.0000000000        1.0000000000
N          1.5590800453        0.9769714469        1.9769714469
C          1.5561432308        0.3484626526       -0.4139962342
H          1.4570686437       -0.9874009351        1.2999992115
C          2.8043642451        0.9238394471        2.5102786295
H          3.0022710644        1.7129064478        3.2524689083
O          3.6511466332        0.0714527378        2.2104016069
H          0.9578263730        1.7566492454        2.2198737061
N          2.8723365054        0.0978743492       -0.6503590527
H          3.2653743694        0.4265642571       -1.5249239211
H          3.4949900855       -0.1212692959        0.1234117771
O          0.7757563370        0.8062442322       -1.2563443045

GDA: C7 conformer, energy in hartrees.
MP2/6-31++G(d,p)=-376.8844440
H         -2.0579865843       -0.4395579421        0.2268936563
C         -0.9715281512       -0.4493573830        0.2260178347
N         -0.4956480199        0.5250726857        1.2001881904
C         -0.5076376157       -0.1165621819       -1.1925362956
H         -0.6125083616       -1.4351125571        0.5262304335
C          0.7461963601        0.4584945489        1.7397180470
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H          0.9412021237        1.2395398074        2.4849785568
O          1.5881071106       -0.3967529367        1.4362848426
H         -1.0941192852        1.2955767332        1.4571746152
N          0.8158989495       -0.3350657195       -1.4148942846
H          1.2017951371       -0.0356567350       -2.2967894491
H          1.4315237293       -0.5541861749       -0.6423719107
O         -1.2948379638        0.3022402118       -2.0478311876

GDA: C7 conformer, energy in hartrees.
MP2/AUG-CC-PVDZ=-376.9635206
H         -2.0769082639       -0.4191207730        0.2305032204
C         -0.9801642836       -0.4358399603        0.2276853592
N         -0.4900620553        0.5330390879        1.2075402080
C         -0.5148082267       -0.1158490379       -1.2003034800
H         -0.6195180552       -1.4321300387        0.5291212562
C          0.7582249238        0.4503038998        1.7409710829
H          0.9705176046        1.2426745497        2.4855542928
O          1.5835477725       -0.4223761636        1.4400540048
H         -1.0664850803        1.3295435663        1.4518141113
N          0.8269405110       -0.2684026827       -1.3937318271
H          1.2146108061       -0.0143793345       -2.2937852292
H          1.4336469876       -0.5006237905       -0.6111150046
O         -1.3077387312        0.2411126105       -2.0774126406

GDA: C7 conformer, energy in hartrees.
MP2/AUG-CC-PVTZ=-377.2858797
H         -2.0603014017       -0.4118031449        0.2310610580
C         -0.9750266067       -0.4288105049        0.2269202877
N         -0.4827607854        0.5337064394        1.1983051753
C         -0.5129930140       -0.1169105957       -1.1950529532
H         -0.6206026961       -1.4162768711        0.5239342275
C          0.7545645958        0.4470077880        1.7308518403
H          0.9627673909        1.2296963648        2.4715390570
O          1.5740890140       -0.4164705739        1.4309961926
H         -1.0598027816        1.3181453802        1.4517480072
N          0.8198557877       -0.2650015272       -1.3826116399
H          1.2074759142       -0.0125643192       -2.2755791982
H          1.4199722694       -0.4913253650       -0.6018662844
O         -1.3001444593        0.2284047546       -2.0668720257

GDA: C7 conformer, energy in hartrees.
LMP2/AVTZ  ENERGY=-377.27197949
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0860560219
N          0.0000000000        1.3768210817        1.5585862036
C          1.2336869085       -0.7811901005        1.5477701783
H         -0.9064176048       -0.4818030963        1.4548340484
C         -0.4291257341        1.7147596663        2.7954866636
H          0.3864280754        2.0986328929        0.9729570367
N          1.2681427124       -1.0205748940        2.8820127807
O          2.0953783393       -1.1485359367        0.7584979870
H         -0.3877555537        2.7956973342        2.9865626456
O         -0.8326188309        0.9094025320        3.6296801638
H          2.0836113439       -1.4685119002        3.2654276641
H          0.5602002000       -0.6306388578        3.4884314861
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1.2 C5 conformer

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GDA: C5 conformer, energy in hartrees.
RHF/6-31G(d)=-375.7486528
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H          0.0000000000        0.0000000000        1.0000000000
C          1.0854513600        0.0000000000        1.0000000000
N          1.5979215983        0.9473720338        1.9473720338
C          1.5905470707        0.3581469812       -0.3872082064
H          1.4012579701       -1.0079605485        1.2499704424
C          1.3040253858        0.8627780745        3.2541961424
H          1.7658231047        1.6518745393        3.8475272692
O          0.6092373566        0.0174473344        3.7405333217
H          2.1822766678        1.6716740384        1.5922363040
N          1.1739888220       -0.4646352172       -1.3699445573
H          1.4714915739       -0.2822119851       -2.3017666267
H          0.5827850512       -1.2452086687       -1.2025689647
O          2.3045336274        1.3022744954       -0.5828254968

GDA: C5 conformer, energy in hartrees.
RHF/6-31+G(d)=-375.7622972
H          0.0000000000        0.0000000000        1.0000000000
C          1.0852054300        0.0000000000        1.0000000000
N          1.5938521761        0.9494074730        1.9494074730
C          1.5904278877        0.3533069819       -0.3881452724
H          1.4027546202       -1.0060165150        1.2544892564
C          1.2982004900        0.8674870310        3.2552774190
H          1.7556869698        1.6559992183        3.8506584115
O          0.6021269087        0.0203226894        3.7431918708
H          2.1792276021        1.6771311122        1.5995612475
N          1.1766874388       -0.4719910263       -1.3702031505
H          1.4746472309       -0.2926652662       -2.3033878969
H          0.5856965777       -1.2534105190       -1.2013409908
O          2.3045659825        1.2987429486       -0.5870367083

GDA: C5 conformer, energy in hartrees.
MP2/6-311++G(d,p)=-377.0287832
H          0.0152577039        0.0021017739        1.0031040439
C          1.1130839951       -0.0092988933        1.0018663236
N          1.6288299794        0.9292211188        1.9672291292
C          1.6244827224        0.3748245724       -0.3817327715
H          1.4241576415       -1.0325668529        1.2408157741
C          1.1020500826        0.9883539012        3.2197387234
H          1.5123963635        1.8218359984        3.8150559192
O          0.2793936848        0.1960567577        3.6562343524
H          2.1771416718        1.6986567215        1.6016054974
N          1.3520852716       -0.5427829240       -1.3585179190
H          1.5079432540       -0.2492632737       -2.3119242072
H          0.6488001245       -1.2479861850       -1.2013361709
O          2.2599606726        1.3993469264       -0.5822213794

GDA: C5 conformer, energy in hartrees.
MP2/6-31G(d)=-376.8003623
H          0.0000000000        0.0000000000        1.0000000000
C          1.0978309600        0.0000000000        1.0000000000
N          1.6045117633        0.9526409512        1.9526409512
C          1.6262767011        0.3727326785       -0.3783874624
H          1.4111595572       -1.0200093189        1.2574225232
C          1.2184190547        0.9063706549        3.2500893865
H          1.6689348791        1.7055724954        3.8641095656
O          0.4471054828        0.0625064977        3.7065133541
H          2.2211675732        1.6712661377        1.5873617467
N          1.2320966561       -0.4565969258       -1.3825829631
H          1.4875471713       -0.2049834219       -2.3280739634
H          0.5143828132       -1.1542702919       -1.2497664921
O          2.3759225369        1.3339134622       -0.5552987204
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GDA: C5 conformer, energy in hartrees.
MP2/6-31+G(d)=-376.8307693
H          0.0000000000        0.0000000000        1.0000000000
C          1.0985052700        0.0000000000        1.0000000000
N          1.5988508760        0.9569825698        1.9569825698
C          1.6208664511        0.3687106184       -0.3806334592
H          1.4168227496       -1.0165246774        1.2629647655
C          1.1125924241        0.9881062728        3.2225614549
H          1.5218755945        1.8123690818        3.8294082779
O          0.3037353189        0.1688117267        3.6710078255
H          2.1701403297        1.7145932242        1.5895021156
N          1.3330691950       -0.5324252070       -1.3629462304
H          1.5384725156       -0.2619208340       -2.3178533408
H          0.6431501689       -1.2591117507       -1.2206893364
O          2.2875019829        1.3889087692       -0.5803877767

GDA: C5 conformer, energy in hartrees.
MP2/6-31++G(d,p)=-376.8822851
H          0.0647180679       -0.0914820097        1.0425429327
C          1.1570078968       -0.0419636194        1.0151659973
N          1.6305712443        0.9292173288        1.9695821464
C          1.6320854071        0.3608107212       -0.3732614677
H          1.5293589719       -1.0429031653        1.2502969452
C          1.0715769379        1.0162450239        3.2034697582
H          1.4584771248        1.8574778154        3.7938685800
O          0.2274535478        0.2259649955        3.6364344568
H          2.2141978902        1.6728830710        1.6064291669
N          1.2900048069       -0.5064379472       -1.3690548988
H          1.4736025709       -0.2152434869       -2.3168702228
H          0.5809806796       -1.2060964601       -1.2220119175
O          2.3155479641        1.3700274739       -0.5666743414

GDA: C5 conformer, energy in hartrees.
MP2/AUG-CC-PVDZ=-376.9618857
H         -0.0539618406        0.0220624218        0.9370405414
C          1.0488570492        0.0347894909        0.9871912049
N          1.5079784388        1.0252628097        1.9341854262
C          1.6271228738        0.3713938244       -0.3848503622
H          1.3692647442       -0.9768590619        1.2918107653
C          1.1404532610        0.9663507639        3.2425043633
H          1.5665302808        1.7896251633        3.8512575374
O          0.4080942841        0.0897337158        3.7120968569
H          2.1128025097        1.7599509121        1.5765257837
N          1.2701018383       -0.4912528748       -1.3815610662
H          1.6196954059       -0.3251916139       -2.3164676202
H          0.6698025217       -1.2857229530       -1.2103958651
O          2.3588418006        1.3483570431       -0.5694202502

GDA: C5 conformer, energy in hartrees.
MP2/AUG-CC-PVTZ=-377.2846959
H         -0.0424693586        0.0215740561        0.9350295033
C          1.0490725118        0.0351975440        0.9874321188
N          1.5049506494        1.0188707137        1.9282966923
C          1.6250459876        0.3715433818       -0.3761000215
H          1.3661565857       -0.9671048094        1.2861678616
C          1.1414527712        0.9624399329        3.2275044511
H          1.5653563131        1.7794656108        3.8274262952
O          0.4157222583        0.0950764683        3.6965966507
H          2.1056378972        1.7467498940        1.5680524037
N          1.2710096816       -0.4842578709       -1.3654808216
H          1.6185244292       -0.3189071880       -2.2940220347
H          0.6748539393       -1.2730201629       -1.1948648973
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O          2.3502695205        1.3408720877       -0.5561206479

GDA: C5 conformer, energy in hartrees.
LMP2/AVTZ  ENERGY=-377.27116646
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0933950748
N          0.0000000000        1.3437449089        1.6062918666
C          1.2413224064       -0.7149125359        1.6086223722
H         -0.8964273230       -0.5389407579        1.4119463141
C         -0.9944469162        2.2091979901        1.3051302266
H          0.7753774998        1.6056055868        2.1985935018
N          1.3647759045       -2.0017698123        1.1958319421
O          2.0572417967       -0.1643485152        2.3367869769
H         -0.8581159697        3.1968863025        1.7686880093
O         -1.9509240322        1.9320901892        0.5919824520
H          2.1633996760       -2.5317102395        1.5005947208
H          0.6837994455       -2.4343958464        0.5983504507
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2 Total energies (hartrees) for GDA at various levels of theory

theory	C7	C5
MP4/6-311G(d,p)//MP2/6-31G(d)	-377.0950851	-377.0926703
MP4/6-311+G(d,p)//MP2/6-31G(d)	-377.1163596	-377.1139256
MP4/6-311++G(d,p)//MP2/6-31G(d)	-377.1170939	-377.1146076
MP4/6-311+G(d,p)//MP2/6-31+G(d)	-377.1162787	-377.1142292
MP4/6-311++G(d,p)//MP2/6-31++G(d,p)	-377.1169125	-377.1149307
MP2/AVTZ//MP2/AVDZ	-377.2848731	-377.2836823
DF-LMP2/AVTZ[a]	-377.2715394	-377.2707224
DF-LMP2/AVQZ[a]	-377.3848000[d]	-377.3839415[e]
DF-LMP2/CBS[a]	-377.4502071	-377.4493078
DF-MP2/AVTZ[a]	-377.2853514	-377.2841809
DF-MP2/AVQZ[a]	-377.3920823	-377.3910545
DF-MP2/CBS[a]	-377.4527245	-377.4517902
LMP2/AVTZ[a]	-377.2719795	-377.2711664
MP2/AVTZ[a]	-377.2858304	-377.2846647
DF-LMP4/AVTZ[a]	-377.3625278	-377.3618197
LMP4/AVTZ[a]	-377.3621420	-377.3614364
MP4/AVTZ[a]	-377.3807875	-377.3792926
DF-LCCSD(T0)/AVTZ[a]	-377.3584803	-377.3577747
DF-LCCSD(T0)/AVQZ[a]	-377.4631071[d]	-377.4623778[e]
DF-LCCSD(T0)/CBS[a]	-377.5222139	-377.5214568
LCCSD(T0)/AVTZ[a]	-377.3581265	-377.3574236
CCSD(T)/AVTZ[a]	-377.3679742	-377.3667432
DF-LMP2/AVTZ[b]	-377.2715394	-377.2707224
LMP2/AVTZ[b]	-377.2719795	-377.2711665
MP2/AVTZ[b]	-377.2858303	-377.2846649
DF-LMP4/AVTZ[b]	-377.3625269	-377.3618186
LMP4/AVTZ[b]	-377.3621413	-377.3614354
MP4/AVTZ[b]	-377.3807854	-377.3792906
DF-LCCSD(T0)/AVTZ[b]	-377.3584815	-377.3577758
LCCSD(T0)/AVTZ[b]	-377.3581278	-377.3574247
CCSD(T)/AVTZ[b]	-377.3679749	-377.3667441
DF-LMP2/AVTZ[c]	-377.2714899	-377.2706909
LMP2/AVTZ[c]	-377.2719298	-377.2711351
MP2/AVTZ[c]	-377.2858797	-377.2846959
DF-LMP4/AVTZ[c]	-377.3623450	-377.3616788
LMP4/AVTZ[c]	-377.3619603	-377.3612971
MP4/AVTZ[c]	-377.3807078	-377.3791973
DF-LCCSD(T0)/AVTZ[c]	-377.3583441	-377.3576829
LCCSD(T0)/AVTZ[c]	-377.3579912	-377.3573327
CCSD(T)/AVTZ[c]	-377.3679339	-377.3666979

[a] Geometry at DF-LMP2/AVTZ. [b] Geometry at LMP2/AVTZ.
[c] Geometry at MP2/AVTZ. [d] Value at THRBP = 0.993.
[e] Value at THRBP = 0.992.

3 Equilibrium structures and total energies for AD at various levels of theory

3.1 C7eq conformer

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AD: C7eq conformer, energy in hartrees.
RHF/6-31G(d)=-492.8615416
H          -2.4207350058       -0.3481775107       -2.0808858463
C          -2.3452090825       -0.4185288630       -1.0030112757
C          -0.8848526891       -0.4345927034       -0.5760084535
N          -0.7877823189       -0.5704500677        0.8716955209
C          -0.1553968538        0.8379850061       -1.0300484829
H          -0.3849797956       -1.2935759974       -1.0009215972
H          -2.8363615609       -1.3292412723       -0.6783065430
H          -2.8617006761        0.4372714837       -0.5860043626
C           0.2620712170       -1.1513754468        1.4875378256
C           0.2038489005       -1.2094465100        2.9973096054
H           0.4851869510       -2.2051183992        3.3137151402
H          -0.7710322801       -0.9644554363        3.4004670559
H           0.9349463308       -0.5159573781        3.3977213340
O           1.2053186711       -1.5950269446        0.8799853334
H          -1.4958598725       -0.1415221544        1.4229105355
N           1.1824074453        0.7192156982       -1.1081969834
C           2.0216245033        1.8611142185       -1.3965637499
H           2.0422309355        2.5692489521       -0.5742971708
H           1.6573708660        2.3733748632       -2.2755493073
H           3.0282751661        1.5120584329       -1.5840309725
H           1.5978175786       -0.1020021934       -0.7243910361
O          -0.7490749829        1.8520023181       -1.2862615593

AD: C7eq conformer, energy in hartrees.
RHF/6-31+G(d)=-492.8746305
H          -2.4806369087       -0.1745033835       -2.0236970690
C          -2.3853190662       -0.2602345912       -0.9482641757
C          -0.9193513230       -0.3675782549       -0.5543993110
N          -0.7974765266       -0.5056731365        0.8914733950
C          -0.1163370090        0.8536369758       -1.0265613435
H          -0.4868619754       -1.2583253435       -0.9884371846
H          -2.9195733520       -1.1458951287       -0.6211756083
H          -2.8451404344        0.6182863955       -0.5119140325
C           0.2134587946       -1.1695028194        1.4882045833
C           0.1701959063       -1.2534337062        2.9963215807
H           1.0871215895       -0.8345420058        3.3922662845
H           0.1347896068       -2.2984938275        3.2797610749
H          -0.6762402429       -0.7380748043        3.4332746875
O           1.1103569884       -1.6799469246        0.8589912936
H          -1.4717946022       -0.0414535508        1.4574579557
N           1.2072576630        0.6510175954       -1.1369252652
C           2.1137468761        1.7332889186       -1.4571725860
H           2.1409318537        2.4794931887       -0.6704183144
H           1.8084331789        2.2176026077       -2.3743947519
H           3.1051783558        1.3213932244       -1.5884763122
H           1.5796242914       -0.2033225860       -0.7812008177
O          -0.6481900368        1.9078675327       -1.2681982070

AD: C7eq conformer, energy in hartrees.
RHF/AUG-CC-PVDZ=-492.9334255
H          -2.4656631657       -0.1956364856       -2.0403668106
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```
C          -2.3805419845       -0.2812255539       -0.9591891032
C          -0.9164811856       -0.3753930614       -0.5555783429
N          -0.7983432749       -0.5081522831        0.8918954649
C          -0.1206477530        0.8506065507       -1.0282015496
H          -0.4702883963       -1.2659005664       -0.9871951557
H          -2.9108522808       -1.1759751344       -0.6347153093
H          -2.8509235025        0.5982596587       -0.5232889784
C           0.2208472681       -1.1587308473        1.4933026506
C           0.1695192697       -1.2406227032        3.0011425706
H           1.1401718894       -0.9515501968        3.3964305971
H          -0.0111465067       -2.2787314060        3.2767553722
H          -0.6063608385       -0.6154556338        3.4384848367
O           1.1199101469       -1.6692006093        0.8679030958
H          -1.4632023170       -0.0325903208        1.4584995694
N           1.2033249617        0.6455401003       -1.1631190358
C           2.1070899811        1.7390046358       -1.4559018807
H           2.1827119508        2.4392776525       -0.6229048793
H           1.7592729130        2.2844708688       -2.3283138713
H           3.0916026922        1.3276065399       -1.6640087835
H           1.5742563159       -0.1992370052       -0.7837256352
O          -0.6553056640        1.9069397575       -1.2504695990

AD: C7eq conformer, energy in hartrees.
B3LYP/6-31G(D)=-495.8551397
H          -2.4971816016       -0.2548767696       -2.0481627145
C          -2.4079173467       -0.2893236598       -0.9593172973
C          -0.9406795057       -0.3888026747       -0.5575528062
N          -0.8214458748       -0.5183335903        0.9000209358
C          -0.1367238358        0.8364200574       -1.0688250255
H          -0.4895728826       -1.2946558517       -0.9763294518
H          -2.9669007977       -1.1537859658       -0.5865750271
H          -2.8541280643        0.6325394255       -0.5734195672
C           0.2349532578       -1.1243605019        1.5057374427
C           0.1720349299       -1.2259929234        3.0197902977
H           1.0494260975       -0.7294815038        3.4454247229
H           0.2270309146       -2.2820582131        3.3015193069
H          -0.7320710600       -0.7892754060        3.4547475162
O           1.1891445802       -1.5779090855        0.8689499188
H          -1.5359864422       -0.0835686924        1.4674532053
N           1.2094584822        0.6487719401       -1.0431964307
C           2.1460984108        1.7010626709       -1.3925208125
H           2.6212140011        2.1354216403       -0.5029091727
H           1.5928436371        2.4847367710       -1.9122350245
H           2.9297233650        1.3116011985       -2.0512479752
H           1.5481640622       -0.1970545924       -0.5895877652
O          -0.6910501980        1.8595805481       -1.4577399666

AD: C7eq conformer, energy in hartrees.
B3LYP/6-31+G(D)=-495.8784103
H          -2.5224165630       -0.1863614570       -2.0240480898
C          -2.4216492306       -0.2575236613       -0.9373904888
C          -0.9500876147       -0.3742854655       -0.5535951217
N          -0.8168116388       -0.5232283785        0.9020337007
C          -0.1335027098        0.8487156624       -1.0480546316
H          -0.5161974399       -1.2796966035       -0.9913828592
H          -2.9744541162       -1.1371690336       -0.5897957899
H          -2.8687312842        0.6482236737       -0.5144147666
C           0.2347090791       -1.1522026595        1.4952291416
C           0.1909654821       -1.2655162646        3.0074729533
H           1.0853567495       -0.7915494089        3.4243541564
H           0.2240364716       -2.3254039131        3.2799487358
H          -0.6973217797       -0.8106667756        3.4572871020
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O          1.1756789967       -1.6140852408        0.8399394958
H         -1.5250827402       -0.0921010200        1.4821156363
N          1.2074833586        0.6444883359       -1.0787462758
C          2.1354947677        1.7114508729       -1.4223678078
H          2.1971521518        2.4689512651       -0.6301876813
H          1.8065677317        2.2067170689       -2.3397700093
H          3.1255559052        1.2769981826       -1.5808198513
H          1.5595424010       -0.2102227134       -0.6528168665
O         -0.6712150179        1.9040390066       -1.3813452410

AD: C7eq conformer, energy in hartrees.
MP2/6-311++G(d,p)=-494.6249598
H         -2.4962263473       -0.1682280558       -2.0507424257
C         -2.4100762476       -0.2561341349       -0.9653731525
C         -0.9491641266       -0.3895254281       -0.5691956161
N         -0.8362830968       -0.5352972917        0.8803182719
C         -0.1339465038        0.8342051910       -1.0185802356
H         -0.5127052151       -1.2931282208       -1.0062293937
H         -2.9699803149       -1.1343479108       -0.6324576371
H         -2.8427050077        0.6476766501       -0.5281661644
C          0.2357331270       -1.1401696757        1.4660350078
C          0.2173896495       -1.1988606814        2.9782071136
H          1.0964579097       -0.6725454508        3.3576118623
H          0.2954077671       -2.2450237337        3.2823884485
H         -0.6837100233       -0.7619175445        3.4142510449
O          1.1576012740       -1.6226753597        0.8052267585
H         -1.5099354682       -0.0531502431        1.4590857075
N          1.1958402991        0.5879581434       -1.1553415169
C          2.1186900081        1.6884703161       -1.3836025839
H          2.1740685088        2.3574477345       -0.5180176627
H          1.7825960468        2.2707258682       -2.2430011030
H          3.1078538570        1.2776723828       -1.5903964633
H          1.5374201004       -0.2717046780       -0.7369583662
O         -0.6535009826        1.9289233245       -1.2211202998

AD: C7eq conformer, energy in hartrees.
MP2/6-31+G(d)=-494.3458296
H         -2.5092522354       -0.1426247643       -2.0479749758
C         -2.4188594956       -0.2327729961       -0.9624128953
C         -0.9588557692       -0.3802001482       -0.5733233161
N         -0.8389338998       -0.5320828020        0.8772547288
C         -0.1295949242        0.8338485762       -1.0151123802
H         -0.5344700071       -1.2891692399       -1.0145824644
H         -2.9839109450       -1.1086258965       -0.6295340931
H         -2.8449132614        0.6739937441       -0.5241501687
C          0.2213728318       -1.1560862144        1.4607856789
C          0.2310458546       -1.1959933138        2.9704967133
H          0.9958181426       -0.5046596041        3.3373045519
H          0.5105142939       -2.2031340504        3.2871670282
H         -0.7327454215       -0.9296622865        3.4124182611
O          1.1404110008       -1.6594848984        0.7885891591
H         -1.5078740125       -0.0383420088        1.4599523880
N          1.2011970998        0.5916841781       -1.1203169753
C          2.1328598251        1.6811317757       -1.3701347583
H          2.1755224564        2.3753264690       -0.5238113510
H          1.8136865923        2.2369414926       -2.2536343223
H          3.1219635197        1.2554843153       -1.5456231862
H          1.5431513056       -0.2845966420       -0.7273573540
O         -0.6468038460        1.9397714936       -1.2374057644

AD: C7eq conformer, energy in hartrees.
MP2/6-31++G(d,p)=-494.4440667
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```
H          -2.4965266280       -0.1758539553       -2.0478495700
C          -2.4108468052       -0.2530464542       -0.9653360764
C          -0.9519690578       -0.3853347548       -0.5698886469
N          -0.8360735657       -0.5280447867        0.8808717484
C          -0.1320213681        0.8322214830       -1.0186094796
H          -0.5178896813       -1.2893778991       -1.0019252188
H          -2.9676773730       -1.1263809023       -0.6266213225
H          -2.8411203300        0.6517423614       -0.5377044020
C           0.2273891074       -1.1435044984        1.4678956490
C           0.2205403453       -1.2023033317        2.9766290336
H           1.0736737132       -0.6382131287        3.3505293763
H           0.3456450114       -2.2399722699        3.2796496103
H          -0.6938552694       -0.8060085214        3.4147671757
O           1.1539782986       -1.6363472111        0.7998558357
H          -1.5110980683       -0.0479964994        1.4588766676
N           1.1990718927        0.5930458328       -1.1338873897
C           2.1238930776        1.6873728323       -1.3795900602
H           2.1899948523        2.3582488403       -0.5211818664
H           1.7811301182        2.2618050344       -2.2367770673
H           3.1045785811        1.2694325151       -1.5914561962
H           1.5418167210       -0.2744477732       -0.7342462067
O          -0.6554247650        1.9350451135       -1.2375500867

AD: C7eq conformer, energy in hartrees.
MP2/6-31G(d)=-494.3109271
H          -2.4820043414       -0.2538883251       -2.0456004479
C          -2.3939879619       -0.2990213332       -0.9581111785
C          -0.9328807259       -0.3984349994       -0.5598870641
N          -0.8149063643       -0.5177945626        0.8925811426
C          -0.1416402824        0.8265792365       -1.0416291049
H          -0.4790505310       -1.3036057424       -0.9772513737
H          -2.9465218589       -1.1683274664       -0.5920792358
H          -2.8333469483        0.6177388688       -0.5583585316
C           0.2520745539       -1.1152469068        1.4877294642
C           0.1901214118       -1.2287819976        2.9943108681
H           1.1902101986       -1.0636620928        3.3972272606
H          -0.1181027802       -2.2435550298        3.2607049349
H          -0.5075909849       -0.5199289158        3.4468389053
O           1.1955723384       -1.5883979860        0.8356463882
H          -1.5085276841       -0.0490832877        1.4628234801
N           1.1993298769        0.6222614556       -1.1023707641
C           2.1011430766        1.7217415718       -1.3932450224
H           2.2840212300        2.3487241310       -0.5134785890
H           1.6526658629        2.3417396045       -2.1696081497
H           3.0500652751        1.3179850376       -1.7496403502
H           1.5544182120       -0.2224934746       -0.6585462555
O          -0.6950949223        1.8916573626       -1.3368353971

AD: C7eq conformer, energy in hartrees.
RHF/CC-PVDZ=-492.9040533
H          -2.4827556525       -0.1345635453       -2.0434324203
C          -2.3944927348       -0.2187133579       -0.9606410517
C          -0.9343854165       -0.3575983590       -0.5609771260
N          -0.8204499156       -0.5167392061        0.8838417585
C          -0.1106264815        0.8537963138       -1.0166384044
H          -0.5088591161       -1.2549261689       -1.0044796941
H          -2.9561573054       -1.0932185983       -0.6286962870
H          -2.8321355814        0.6811963388       -0.5283390827
C           0.2003210657       -1.1806916127        1.4724978132
C           0.1788574817       -1.2104703354        2.9824065867
H           0.6980157429       -0.3258704298        3.3578209411
H           0.7154193835       -2.0929401442        3.3211174740
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H          -0.8350152767        -1.2134957540         3.3824293645
O           1.0807396828        -1.7039835990         0.8388734962
H          -1.4556858701        -0.0040550106         1.4581192704
N           1.2087937354         0.6127617994        -1.1551866182
C           2.1461861368         1.6805241057        -1.4236185212
H           2.3852079501         2.2589796146        -0.5267713432
H           1.7234573358         2.3573080028        -2.1614404599
H           3.0663680373         1.2528558460        -1.8194553507
H           1.5556685958        -0.2485287668        -0.7821049112
O          -0.6191265941         1.9219860909        -1.2243146540

AD: C7eq conformer, energy in hartrees.
DF-LMP2/AVTZ  ENERGY=-494.94308840
H           0.0000000000         0.0000000000         0.0000000000
C           0.0000000000         0.0000000000         1.0879380552
C           0.0000000000         1.4254112884         1.6089100163
H           0.8824753274        -0.5296946564         1.4449710329
H          -0.8997799558        -0.5223716816         1.4114022501
N           0.0195554400         1.4189104054         3.0700814611
C          -1.2323268426         2.2006144286         1.1085506870
H           0.8993448882         1.9573975694         1.2930295655
C           0.5192009414         2.4481754486         3.8010318192
H          -0.4104695365         0.6425646516         3.5468148691
N          -1.1200012546         3.5431544158         1.2292282143
O          -2.2259579928         1.6374596673         0.6528346311
C           0.4928149873         2.2718798967         5.3012988088
O           0.9764419866         3.4661940904         3.2743236170
C          -2.2465410442         4.4065938515         0.9249711794
H          -0.3291966031         3.8947665102         1.7557689528
H          -0.0706035499         3.0950518703         5.7368367685
H           1.5142888323         2.3356887834         5.6722768975
H           0.0541568573         1.3264975444         5.6143310979
H          -3.0692548225         4.2523172574         1.6246388793
H          -2.6121365882         4.1946711372        -0.0775316742
H          -1.9165604364         5.4406558153         0.9776418552
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3.2 C5 conformer

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AD: C5 conformer, energy in hartrees.
RHF/6-31G(d)=-492.8608896
H          -1.8363359122        -0.0924401645        -1.9381020107
C          -1.7756459311        -0.1138218366        -0.8548128962
C          -0.3225457095        -0.2494033698        -0.3797448808
N          -0.2232426008        -0.3144368860         1.0574191871
C           0.4993802781         0.9507951609        -0.8407541420
H           0.0970005709        -1.1598218725        -0.7895442073
H          -2.3471496099        -0.9592277763        -0.4953604561
H          -2.2145189850         0.7992023930        -0.4673818604
C          -0.4356866321        -1.4559575395         1.7420499087
C          -0.2947316755        -1.3595853119         3.2457062846
H           0.2635805155        -2.2173317231         3.5967329936
H          -1.2838107971        -1.4040733219         3.6884783123
H           0.1937571463        -0.4499059192         3.5729674070
O          -0.7368051414        -2.4888205826         1.2016187632
H           0.0495324929         0.5239323120         1.5191834854
N           0.8935835499         0.9271088583        -2.1264797239
C           1.6685418814         2.0051606969        -2.7053002486
H           2.6796190457         2.0239600606        -2.3150720821
H           1.2004519357         2.9545881490        -2.4886943903
H           1.7065555105         1.8669444531        -3.7773549780
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H          0.7571442779        0.0983897782       -2.6570217251
O          0.7375443786        1.8718147107       -0.1026526240

AD: C5 conformer, energy in hartrees.
RHF/6-31+G(d)=-492.8741595
H         -1.8753284922       -0.0281944863       -1.9235100865
C         -1.8064567592       -0.0544398125       -0.8404894999
C         -0.3533391374       -0.2314848698       -0.3785046485
N         -0.2466168352       -0.3094970352        1.0591539832
C          0.4966561872        0.9485404120       -0.8405387046
H          0.0381538630       -1.1515778165       -0.7936186045
H         -2.3983869602       -0.8861601945       -0.4808981403
H         -2.2199324651        0.8677193150       -0.4464907237
C         -0.4371903280       -1.4589589871        1.7361258861
C         -0.2654174032       -1.3865622655        3.2369426179
H          0.4526206447       -2.1391211516        3.5385744250
H         -1.2130433743       -1.6284103434        3.7038706784
H          0.0643482216       -0.4156842463        3.5859192905
O         -0.7341789808       -2.4918793401        1.1873872290
H          0.0286177597        0.5240647811        1.5302469228
N          0.9234622938        0.9018757573       -2.1135375984
C          1.6942397680        1.9796826936       -2.7020230422
H          2.6329322010        2.1145098066       -2.1800357092
H          1.1422879296        2.9093420332       -2.6621912153
H          1.8951936135        1.7312936805       -3.7351189125
H          0.7447821572        0.0876509116       -2.6548397471
O          0.7340393217        1.8777860441       -0.1086745445

AD: C5 conformer, energy in hartrees.
RHF/AUG-CC-PVDZ=-492.9330835
H         -1.8681132552       -0.0445089469       -1.9274698860
C         -1.8042991438       -0.0667612252       -0.8394732159
C         -0.3500743490       -0.2318442517       -0.3764095747
N         -0.2389825908       -0.3084474613        1.0621817729
C          0.4901923560        0.9532502547       -0.8425734012
H          0.0505471228       -1.1524717093       -0.7946079021
H         -2.3916498043       -0.9055902582       -0.4752114160
H         -2.2235778923        0.8592869930       -0.4471780680
C         -0.4340690953       -1.4588955107        1.7391985138
C         -0.2690587798       -1.3859860015        3.2404184635
H          0.4543232419       -2.1403744445        3.5426356334
H         -1.2240073219       -1.6335881576        3.7009859149
H          0.0563568373       -0.4078691053        3.5887011919
O         -0.7280352485       -2.4912603178        1.1882148199
H          0.0305566426        0.5245327197        1.5358237531
N          0.9128639811        0.9068855992       -2.1196325296
C          1.6990213411        1.9770118958       -2.7028221692
H          2.6783003749        2.0525982856       -2.2323117068
H          1.1870284525        2.9282675811       -2.5845973287
H          1.8276443933        1.7721773518       -3.7624631185
H          0.7761971829        0.0703028158       -2.6377731866
O          0.7204040383        1.8872001855       -0.1150161050

AD: C5 conformer, energy in hartrees.
B3LYP/6-31G(D)=-495.8528906
H         -1.7262666460       -0.2163753818       -2.0378790890
C         -1.7189110892       -0.1973758079       -0.9419717574
C         -0.2824783055       -0.2708296435       -0.3863994452
N         -0.2608403493       -0.2944890283        1.0622716421
C          0.5500137926        0.9448400997       -0.8262763385
H          0.1830748364       -1.1954115362       -0.7514170771
H         -2.2810968616       -1.0598763055       -0.5760062979
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H          -2.2119652998        0.7211103572       -0.6070745016
C          -0.5067174038       -1.4321676428        1.7697911105
C          -0.3698503041       -1.3078123083        3.2801542749
H           0.3898442022       -2.0163684112        3.6250042420
H          -1.3176622968       -1.5952300649        3.7456612227
H          -0.0984464330       -0.3021207848        3.6153491250
O          -0.8208757645       -2.4887893623        1.2278447938
H           0.0686016585        0.5579551778        1.5003613252
N           0.9255814932        0.9412536691       -2.1331857392
C           1.6704808004        2.0278616218       -2.7465933305
H           2.6348941648        1.6763703549       -3.1308170848
H           1.8457690603        2.7795176830       -1.9762019425
H           1.1042723921        2.4804221036       -3.5689399492
H           0.6819149366        0.1414143701       -2.7000941290
O           0.8232074316        1.8530571170       -0.0445665747

AD: C5 conformer, energy in hartrees.
B3LYP/6-31+G(D)=-495.8766781
H          -1.8664927505       -0.0680199539       -1.9596201012
C          -1.8066387406       -0.0754707457       -0.8648715871
C          -0.3490072741       -0.2389838117       -0.3863357596
N          -0.2558285124       -0.3072824033        1.0612160857
C           0.5162570972        0.9467209644       -0.8406837507
H           0.0495430560       -1.1770407848       -0.7920912790
H          -2.4013759475       -0.9138926421       -0.4918341778
H          -2.2315407676        0.8605602980       -0.4862560605
C          -0.4625999928       -1.4627632195        1.7530251393
C          -0.2754372160       -1.3778195857        3.2587775570
H           0.4893639000       -2.1010989641        3.5598675860
H          -1.2113310937       -1.6674326084        3.7476550171
H           0.0161459375       -0.3822567794        3.6085090209
O          -0.7852142406       -2.5132697667        1.1962030058
H           0.0664891098        0.5382024707        1.5198088594
N           0.9176849238        0.9227283118       -2.1365172955
C           1.7051096081        2.0023474250       -2.7196765204
H           2.6973445478        2.0604651778       -2.2586416894
H           1.2010864640        2.9615634898       -2.5698436015
H           1.8147508805        1.8156009379       -3.7903017996
H           0.7174891965        0.1053557414       -2.6960307958
O           0.7926432027        1.8752305288       -0.0793933784

AD: C5 conformer, energy in hartrees.
MP2/6-311++G(d,p)=-494.6223094
H          -1.9241863192       -0.0315238092       -1.8705550680
C          -1.8193933412       -0.0630883634       -0.7813540988
C          -0.3483232333       -0.2303932220       -0.3779701881
N          -0.1927562408       -0.3117487363        1.0585417835
C           0.4663059906        0.9681645113       -0.8519562554
H           0.0412550626       -1.1592397270       -0.8096528468
H          -2.3938552997       -0.9082450745       -0.3949953456
H          -2.2129954662        0.8669066094       -0.3604490858
C          -0.4168447782       -1.4771305857        1.7309981038
C          -0.2596657257       -1.4000648186        3.2363792098
H           0.4427767699       -2.1744141085        3.5520038280
H          -1.2267541390       -1.6162814374        3.6970617373
H           0.0937853682       -0.4254557807        3.5805089811
O          -0.7249486158       -2.5169389087        1.1530070395
H           0.0358512891        0.5477405765        1.5408531751
N           0.9433983919        0.8830735409       -2.1207896081
C           1.7247318477        1.9684192473       -2.6941965668
H           2.6800137433        2.0886414658       -2.1751219262
H           1.1681437849        2.9035457214       -2.6118373656
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H          1.9064817652        1.7489326641       -3.7469896357
H          0.9202633008       -0.0121940222       -2.5841359867
O          0.6166811811        1.9640479932       -0.1470516541

AD: C5 conformer, energy in hartrees.
MP2/6-31+G(d)=-494.3429784
H         -1.9317075053       -0.0242865453       -1.8952473527
C         -1.8384324190       -0.0514111882       -0.8040751045
C         -0.3756974227       -0.2242004427       -0.3800244090
N         -0.2420057472       -0.2953994287        1.0605485204
C          0.4607895690        0.9587868654       -0.8482394193
H          0.0128768795       -1.1633598442       -0.7930332456
H         -2.4216165244       -0.8933361856       -0.4218723141
H         -2.2354481492        0.8816224464       -0.3922176583
C         -0.3987451774       -1.4702738256        1.7318614138
C         -0.2449670497       -1.4022069076        3.2345372391
H          0.4360078016       -2.1956902739        3.5510366410
H         -1.2181981672       -1.5937044778        3.6953948763
H          0.1319611968       -0.4371204467        3.5835338481
O         -0.6695670355       -2.5309851857        1.1465283207
H          0.0031387879        0.5695158353        1.5353279412
N          0.9570690266        0.8724562227       -2.1067395318
C          1.7259743808        1.9645666935       -2.6876956966
H          2.6698991302        2.1068261174       -2.1540942062
H          1.1519901661        2.8914936547       -2.6286723697
H          1.9282885352        1.7258579373       -3.7326266681
H          0.8824593698       -0.0054497953       -2.6057535187
O          0.6209888150        1.9618185419       -0.1336062001

AD: C5 conformer, energy in hartrees.
MP2/6-31++G(d,p)=-494.4413837
H         -1.9329854704       -0.0200688291       -1.8932714853
C         -1.8451375144       -0.0441710038       -0.8059917406
C         -0.3844217711       -0.2197676072       -0.3786378202
N         -0.2536166631       -0.2915011251        1.0611764789
C          0.4558694796        0.9605685159       -0.8461775968
H          0.0011840148       -1.1563385762       -0.7896149242
H         -2.4286320431       -0.8805449989       -0.4243076743
H         -2.2381598094        0.8877106984       -0.3989706227
C         -0.3961231362       -1.4706019552        1.7290086629
C         -0.2353657415       -1.4024651720        3.2306405565
H          0.4847108618       -2.1590233413        3.5357930675
H         -1.1915820012       -1.6432912279        3.6928767561
H          0.0942440215       -0.4247933688        3.5783336623
O         -0.6557008860       -2.5320667079        1.1418477800
H         -0.0129981045        0.5682543358        1.5366098588
N          0.9581843500        0.8666998175       -2.1022549681
C          1.7339262474        1.9527901361       -2.6814848723
H          2.6808137157        2.0816151965       -2.1578826377
H          1.1717007555        2.8812886141       -2.6109494829
H          1.9234872313        1.7213761915       -3.7261110665
H          0.8929113703       -0.0136662306       -2.5881349320
O          0.6120566694        1.9661883589       -0.1357183089

AD: C5 conformer, energy in hartrees.
MP2/6-31G(d)=-494.3081649
H         -1.7482781491       -0.2045060006       -1.9907117642
C         -1.7178278941       -0.1989579312       -0.8967119339
C         -0.2777576972       -0.2673113851       -0.3785970976
N         -0.2309653246       -0.2939489766        1.0650770663
C          0.5184056544        0.9544044278       -0.8268497235
H          0.1917201505       -1.1867385673       -0.7513484670
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H          -2.2652993211       -1.0663180871       -0.5230793214
H          -2.1949232471        0.7160286505       -0.5354295491
C          -0.4533337216       -1.4455994047        1.7550171111
C          -0.3672936885       -1.3286613628        3.2620054639
H           0.1017178324       -2.2327687291        3.6529742583
H          -1.3785301074       -1.2686471271        3.6739934387
H           0.1972958938       -0.4517283383        3.5878029271
O          -0.7436837019       -2.5054726940        1.1881079960
H           0.0650533541        0.5673446263        1.5127070684
N           0.9199336880        0.9292364390       -2.1241764064
C           1.6462423977        2.0285460992       -2.7347953506
H           2.6849385010        1.7528533491       -2.9387981822
H           1.6297938902        2.8567215452       -2.0275963536
H           1.1644501440        2.3341909315       -3.6667757646
H           0.7681322666        0.0842471142       -2.6591687792
O           0.7275011948        1.9051959110       -0.0632686143

AD: C5 conformer, energy in hartrees.
RHF/CC-PVDZ=-492.9031879
H          -1.7814164682       -0.1582426861       -1.9876609863
C          -1.7525756896       -0.1748677875       -0.8965315643
C          -0.3119517368       -0.2558006244       -0.3779156558
N          -0.2515897401       -0.3083772866        1.0623078334
C           0.4924481881        0.9605094185       -0.8286016474
H           0.1522936415       -1.1599496872       -0.7731164984
H          -2.3069338472       -1.0449950847       -0.5481898928
H          -2.2387891082        0.7286358317       -0.5233396811
C          -0.4220289761       -1.4608216360        1.7473044321
C          -0.3085457688       -1.3436960523        3.2499952901
H          -0.0439846227       -2.3157150828        3.6583838838
H          -1.2795181085       -1.0497719890        3.6544346115
H           0.4281016327       -0.5984276643        3.5510039068
O          -0.6743102889       -2.5023050212        1.2030116888
H           0.0197966714        0.5340385367        1.5245921205
N           0.8496468684        0.9642551939       -2.1292410484
C           1.6424310858        2.0295705020       -2.7062822047
H           2.7115869643        1.8870308920       -2.5316911726
H           1.3457467049        2.9755629663       -2.2626889906
H           1.4620645232        2.0673989997       -3.7797976015
H           0.7383594338        0.1216302150       -2.6503177255
O           0.7452640475        1.8638420812       -0.0768731100

AD: C5 conformer, energy in hartrees.
DF-LMP2/AVTZ  ENERGY=-494.94115043
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0904667840
C           0.0000000000        1.4304165522        1.6432832840
H           0.8932255758       -0.5133877736        1.4414499052
H          -0.8842058518       -0.5320060447        1.4416983170
N           0.0560403240        1.4427288083        3.0868331890
C          -1.2789180434        2.1587384097        1.2387221597
H           0.8760997454        1.9614375535        1.2614530455
C           1.2274434805        1.2637078113        3.7519877490
H          -0.8033035037        1.6703948965        3.5657714777
N          -1.3232951823        2.5878877109       -0.0433146973
O          -2.2215677776        2.3041298913        2.0165223481
C           1.1425317615        1.3385772770        5.2604189917
O           2.2869067149        1.0503325263        3.1640288990
C          -2.5057728991        3.2490232149       -0.5693023679
H          -0.5017372400        2.4998434107       -0.6155990774
H           1.8264694705        2.1112706146        5.6067621380
H           1.4785116009        0.3888206442        5.6730145676
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H          0.1385377072        1.5538371413        5.6208352868
H         -2.6908001031        4.1868956038       -0.0472024694
H         -3.3786259823        2.6110588698       -0.4445668127
H         -2.3517014663        3.4477765366       -1.6263218355
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3.3 C7ax conformer

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AD: C7ax conformer, energy in hartrees.
RHF/6-31G(d)=-492.8570485
H         -1.5098434642       -1.1692302482       -2.1955167959
C         -1.5002875759       -1.1384428988       -1.1114942940
C         -0.0498448160       -1.0781291559       -0.6236370408
N          0.0754548742       -1.1489846044        0.8325069372
C          0.7137535191        0.0876783542       -1.2663922669
H          0.4654884232       -1.9520999715       -0.9929287653
H         -1.9748532468       -2.0401782247       -0.7400019150
H         -2.0743848804       -0.2860610108       -0.7800648353
C         -0.5420315932       -0.3695608394        1.7426031415
C         -0.3309136033       -0.7571273236        3.1901627521
H         -0.2580991907        0.1438772510        3.7830675303
H          0.5501134700       -1.3676630084        3.3470926060
H         -1.2004968752       -1.3113766601        3.5274401523
O         -1.2417911462        0.5691371770        1.4487263526
H          0.6792472403       -1.8581430534        1.1778924488
N          0.4390844219        1.3221485703       -0.8219792806
C          1.0795133527        2.4827983912       -1.3990572661
H          0.8304783474        2.5882574096       -2.4481778707
H          2.1566850729        2.4135841430       -1.3136115832
H          0.7401559613        3.3613899469       -0.8671260173
H         -0.2375852886        1.4354389725       -0.0992433943
O          1.4930641034       -0.1357924862       -2.1569295165

AD: C7ax conformer, energy in hartrees.
RHF/6-31+G(d)=-492.8700549
H         -1.2875293585       -1.3325642849       -2.2538723181
C         -1.3568524888       -1.2623326699       -1.1735457643
C          0.0498337608       -1.0984946174       -0.5903285267
N          0.0795194204       -1.1196471298        0.8733132930
C          0.7908320878        0.0914414300       -1.2163327066
H          0.6383485488       -1.9518327020       -0.8922637589
H         -1.8024500064       -2.1784174418       -0.8004148418
H         -2.0045121647       -0.4366943882       -0.9183190517
C         -0.6400970980       -0.3525930906        1.7166693401
C         -0.5008598744       -0.6687269720        3.1888807751
H         -0.3536653028        0.2568654193        3.7295750368
H          0.3114720795       -1.3497647709        3.4111585617
H         -1.4306132069       -1.1093720720        3.5313166701
O         -1.3695668659        0.5357893563        1.3419793979
H          0.6972630716       -1.7837253746        1.2802399034
N          0.4148713904        1.3217423741       -0.8447864093
C          1.0335925839        2.5018266198       -1.4098999730
H          0.5846173083        3.3731501427       -0.9526513508
H          0.8821968827        2.5463324555       -2.4814969367
H          2.0991758197        2.5105490938       -1.2175928552
H         -0.3191669007        1.4200109251       -0.1768619345
O          1.6527460816       -0.1165303452       -2.0358749201

AD: C7ax conformer, energy in hartrees.
RHF/AUG-CC-PVDZ=-492.9287549
H         -1.2651771171       -1.3442862631       -2.2608575861
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C          -1.3468402845       -1.2710540023       -1.1769791989
C           0.0555792798       -1.0994302185       -0.5851860725
N           0.0817741119       -1.1158969155        0.8791917253
C           0.7889739057        0.0906108860       -1.2206184736
H           0.6529400436       -1.9532366656       -0.8856581643
H          -1.7931722119       -2.1918104125       -0.8026436908
H          -1.9993394392       -0.4412258661       -0.9262995093
C          -0.6437559075       -0.3485799699        1.7192185235
C          -0.5083855497       -0.6642393226        3.1917459042
H          -0.3839188305        0.2689276372        3.7347853851
H           0.3198974012       -1.3336130907        3.4153265353
H          -1.4375775668       -1.1264660168        3.5232868893
O          -1.3750723430        0.5367817480        1.3412009427
H           0.6975402162       -1.7759392333        1.2934840107
N           0.4400954757        1.3211144748       -0.8191654710
C           1.0391875494        2.5012420918       -1.4063104883
H           0.6440049386        3.3760393573       -0.8962669617
H           0.8105013189        2.5751229154       -2.4686533151
H           2.1211972960        2.4824537316       -1.2933544352
H          -0.2924274431        1.4131364231       -0.1490864518
O           1.6205586332       -0.1163970253       -2.0706343992

AD: C7ax conformer, energy in hartrees.
B3LYP/6-31G(D)=-495.8509943
H          -1.4108334719       -1.2344392782       -2.2423230641
C          -1.4293016991       -1.2228634120       -1.1476969041
C           0.0088826563       -1.1145890842       -0.6171873051
N           0.0737016893       -1.1615403323        0.8561662626
C           0.7730426064        0.0737446246       -1.2553640527
H           0.5722502840       -1.9863912049       -0.9557050415
H          -1.8905887448       -2.1532000588       -0.7991537156
H          -2.0417842097       -0.3842978075       -0.8123400499
C          -0.5810798750       -0.3480795690        1.7271072919
C          -0.4250535394       -0.6934699045        3.1997745846
H          -0.0810949405        0.1962362462        3.7350328963
H           0.2667867776       -1.5188354897        3.3936209632
H          -1.4086110102       -0.9560993478        3.6026268630
O          -1.2700911868        0.6128850363        1.3732615927
H           0.6631956815       -1.8799562826        1.2504399005
N           0.3878393197        1.3087975370       -0.8472189442
C           0.9959866914        2.5206208211       -1.3643028683
H           0.2409392014        3.1762193020       -1.8142304926
H           1.7208930832        2.2326175581       -2.1269771668
H           1.5110467193        3.0765471805       -0.5709507149
H          -0.3220079798        1.3653639004       -0.1188281599
O           1.6318612497       -0.1449782872       -2.1054900831

AD: C7ax conformer, energy in hartrees.
B3LYP/6-31+G(D)=-495.8744435
H          -1.2891101188       -1.3442755724       -2.2705834999
C          -1.3530996963       -1.3002112276       -1.1779796983
C           0.0588472757       -1.1217026000       -0.5954913222
N           0.0740129008       -1.1456930239        0.8810567848
C           0.7965034925        0.0847952200       -1.2272109327
H           0.6661728346       -1.9780378434       -0.8964990573
H          -1.7899711907       -2.2391240541       -0.8194694435
H          -2.0144292009       -0.4781417469       -0.8960214468
C          -0.6322508958       -0.3425572448        1.7228470333
C          -0.5174884513       -0.6595119724        3.2037037152
H          -0.2017581265        0.2440660166        3.7341811100
H           0.1801377243       -1.4716872333        3.4317188174
H          -1.5097300234       -0.9308624206        3.5796298165
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O          -1.3329747263        0.5960615912        1.3267766120
H           0.6692833378       -1.8443734477        1.3040791140
N           0.4003106654        1.3165652521       -0.8350887156
C           1.0031401478        2.5192090447       -1.3896122956
H           0.5561551891        3.3878730686       -0.9004853516
H           0.8296511267        2.5836832094       -2.4697096365
H           2.0855685144        2.5263542410       -1.2212412838
H          -0.3352288093        1.3849829313       -0.1337135148
O           1.6703600442       -0.1106478493       -2.0744267503

AD: C7ax conformer, energy in hartrees.
MP2/6-311++G(d,p)=-494.6212425
H          -1.2964555624       -1.3083069501       -2.2543739374
C          -1.3554575341       -1.2676060340       -1.1626858172
C           0.0593776955       -1.1188380634       -0.5960851827
N           0.0867090659       -1.1415480197        0.8719196286
C           0.7991947944        0.0775855806       -1.2169071673
H           0.6538912291       -1.9812862686       -0.9068112176
H          -1.8041346093       -2.1972630305       -0.8000414540
H          -1.9922562658       -0.4316662103       -0.8714553493
C          -0.6304224530       -0.3399704034        1.7068576719
C          -0.5064961698       -0.6571634067        3.1831234594
H          -0.2130638410        0.2535104478        3.7094276567
H           0.2118630918       -1.4509629785        3.3993883204
H          -1.4915235430       -0.9546901645        3.5513010642
O          -1.3423799254        0.5851330450        1.3090346121
H           0.6802936521       -1.8347040367        1.3019929705
N           0.3745832554        1.3029569071       -0.8336817814
C           0.9923040608        2.4981688677       -1.3812439614
H           0.4980546821        3.3705060044       -0.9515614906
H           0.8880620224        2.5208386435       -2.4692722705
H           2.0590669213        2.5301984241       -1.1422780784
H          -0.3586072457        1.3609060250       -0.1331426735
O           1.6904750325       -0.1051332153       -2.0464336730

AD: C7ax conformer, energy in hartrees.
MP2/6-31+G(d)=-494.3419803
H          -1.2650683231       -1.3465215144       -2.2695024052
C          -1.3362148784       -1.2906390185       -1.1785261914
C           0.0702921546       -1.1197364894       -0.6008122407
N           0.0871039520       -1.1430227787        0.8693563675
C           0.7998795372        0.0856459050       -1.2096222429
H           0.6803816606       -1.9743886201       -0.9068837050
H          -1.7771397757       -2.2217525136       -0.8085591778
H          -1.9881561082       -0.4599116432       -0.9048044745
C          -0.6462997262       -0.3566246937        1.7026477747
C          -0.5027761266       -0.6354518399        3.1815983841
H          -0.0471335825        0.2364736252        3.6591673056
H           0.0972432655       -1.5217430256        3.4033948770
H          -1.5024496410       -0.7616247454        3.6044219269
O          -1.3893363301        0.5556937442        1.2946522536
H           0.7149561254       -1.8120807348        1.3001269050
N           0.3861042158        1.3083298066       -0.8109610755
C           0.9937174833        2.5106063670       -1.3581824744
H           0.5477849603        3.3747583282       -0.8635605991
H           0.8209707585        2.5761644695       -2.4363180212
H           2.0733820376        2.5053687642       -1.1863616433
H          -0.3641848352        1.3667142263       -0.1228071583
O           1.6925070326       -0.0908696436       -2.0571146198

AD: C7ax conformer, energy in hartrees.
MP2/6-31++G(d,p)=-494.4405893
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```
H          -1.2874559788       -1.3269233711       -2.2494015992
C          -1.3502169078       -1.2787648085       -1.1620184335
C           0.0615205961       -1.1176253287       -0.5960194881
N           0.0899308044       -1.1378711116        0.8728881566
C           0.7954033412        0.0795916392       -1.2155801676
H           0.6601564249       -1.9746245910       -0.9033196641
H          -1.7885242181       -2.2074115352       -0.7956368556
H          -1.9924184792       -0.4493923512       -0.8771882994
C          -0.6336799621       -0.3441777208        1.7078017569
C          -0.5133141884       -0.6490835698        3.1832441882
H          -0.2391805116        0.2663264692        3.7036910629
H           0.2160849400       -1.4258607522        3.4059883275
H          -1.4909006509       -0.9619531056        3.5472240836
O          -1.3630702821        0.5792363289        1.3023357793
H           0.7003490549       -1.8172923452        1.3005973204
N           0.3944153897        1.3061956654       -0.8148611307
C           1.0041751217        2.5007396728       -1.3729001595
H           0.5709965627        3.3671011211       -0.8799945513
H           0.8223197975        2.5628291614       -2.4456425519
H           2.0813233255        2.4894666154       -1.2113284960
H          -0.3474293389        1.3689142492       -0.1245696593
O           1.6781862458       -0.1059276723       -2.0703075890

AD: C7ax conformer, energy in hartrees.
MP2/6-31G(d)=-494.3068732
H          -1.3803873059       -1.2256244391       -2.2371167376
C          -1.4080777664       -1.2158842464       -1.1438327632
C           0.0195187524       -1.1165012357       -0.6085984706
N           0.0714962829       -1.1493523004        0.8593641332
C           0.7941731291        0.0639249149       -1.2116976341
H           0.5850565813       -1.9919213363       -0.9383991151
H          -1.8717239292       -2.1436209945       -0.7968545360
H          -2.0127297854       -0.3738610854       -0.8093090913
C          -0.6045068240       -0.3294815472        1.7071762053
C          -0.4790126802       -0.6728363193        3.1763967180
H          -0.5060045085        0.2539249834        3.7502778711
H           0.4375128859       -1.2202535529        3.4102462915
H          -1.3363005006       -1.2831952072        3.4745670661
O          -1.3165239124        0.6142131346        1.3284273658
H           0.6829808770       -1.8407052994        1.2735285858
N           0.3224156325        1.2961732704       -0.9094622613
C           1.0086060940        2.4761816549       -1.4019040998
H           0.4050094612        3.3528036030       -1.1637836006
H           1.1358955065        2.4041816585       -2.4836307008
H           1.9997257522        2.5848183028       -0.9497562960
H          -0.3984938288        1.3711975435       -0.1943765748
O           1.7562578070       -0.1327019212       -1.9646706157

AD: C7ax conformer, energy in hartrees.
RHF/CC-PVDZ=-492.8991626
H          -1.3953191842       -1.2381526152       -2.2484678611
C          -1.4336108962       -1.1938072215       -1.1584226450
C          -0.0100892656       -1.0982192743       -0.6093389825
N           0.0554424620       -1.1375527742        0.8533813152
C           0.7828938659        0.0692122366       -1.2135396593
H           0.5431727055       -1.9728871109       -0.9393762830
H          -1.9073561316       -2.1075330133       -0.7945376099
H          -2.0457514484       -0.3462645469       -0.8626122453
C          -0.6053756294       -0.3352679473        1.7165984673
C          -0.4423482933       -0.6846895676        3.1782016464
H          -0.6295540312        0.2055337477        3.7726542123
H           0.5485687905       -1.0799125598        3.4031086734
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H          -1.1840343962       -1.4414498259        3.4423266556
O          -1.3012077660        0.5843673976        1.3662957081
H           0.6558484891       -1.8298985140        1.2447024193
N           0.3232756019        1.3079227066       -0.9621131744
C           1.0376042914        2.4776095237       -1.4222438389
H           0.3829496305        3.3436865520       -1.3367135160
H           1.3250172075        2.3516522389       -2.4635399909
H           1.9443381435        2.6636581265       -0.8404938346
H          -0.3866433984        1.4108688984       -0.2647438186
O           1.7416193584       -0.1544820728       -1.9036349224

AD: C7ax conformer, energy in hartrees.
DF-LMP2/AVTZ  ENERGY=-494.93924342
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0897714023
C           0.0000000000        1.4473339233        1.5854467615
H           0.8956144252       -0.5131530681        1.4395725413
H          -0.8747518766       -0.5376995964        1.4460216906
N           0.0847204433        1.5421706834        3.0475205886
C          -1.1563235028        2.2453098540        0.9619099786
H           0.8923841455        1.9465561891        1.2107259657
C          -0.7363143636        0.9447493023        3.9480269944
H           0.8362291275        2.0982989914        3.4188561757
N          -2.3854052013        2.0066677543        1.4620812358
O          -0.9406568677        3.0221169197        0.0305223284
C          -0.3543221234        1.1215890042        5.4008025512
O          -1.7347377777        0.2946670097        3.6251666262
C          -3.5469152359        2.6726471146        0.9023815420
H          -2.4768730548        1.3162334582        2.1990221521
H          -1.2087158113        1.5330912120        5.9344610505
H           0.5104156033        1.7657533500        5.5467703790
H          -0.1434511790        0.1387037320        5.8194701427
H          -4.4227884338        2.3793758404        1.4749382347
H          -3.6880283503        2.3975142954       -0.1427754679
H          -3.4268800352        3.7540046856        0.9518794577
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3.4 β_2 conformer

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AD: Beta2 conformer, energy in hartrees.
RHF/6-31G(d)=-492.8574375
H          -2.1454137488       -0.1112613066       -2.0909476884
C          -2.0578297976       -0.2329704206       -1.0212106077
C          -0.5884668719       -0.2436742851       -0.6039266915
N          -0.4308384526       -0.4148890228        0.8307210213
C           0.1415919222        0.9959491877       -1.1302156142
H          -0.0970035199       -1.0926481868       -1.0596130704
H          -2.5265356004       -1.1659303896       -0.7289871982
H          -2.5916459027        0.5856467256       -0.5468326092
C          -0.0934312778       -1.6136474866        1.3899616903
C          -0.2681144176       -1.6890358608        2.8916653064
H           0.3706151211       -2.4688182903        3.2799120053
H          -1.2991933775       -1.9450328790        3.1166620081
H          -0.0378799830       -0.7488920856        3.3802470349
O           0.3113122119       -2.5396119425        0.7471273315
H          -0.9110985146        0.2365067194        1.4124718687
N           1.1563567798        1.4623111219       -0.3776387844
C           2.0186567786        2.5207144049       -0.8567134219
H           2.6334722357        2.8666195667       -0.0361335027
H           1.4207754704        3.3435966376       -1.2203779846
H           2.6621551630        2.1844126540       -1.6626114991
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H          1.4377891658        0.9277789379        0.4099770098
O         -0.1749500637        1.4936186882       -2.1774655816

AD: Beta2 conformer, energy in hartrees.
RHF/6-31+G(d)=-492.8707682
H         -2.3073856938        0.1589479520       -2.0551034911
C         -2.2279159343        0.0215969165       -0.9865091184
C         -0.7752148837       -0.2572802824       -0.5995454083
N         -0.6623582452       -0.4487947925        0.8374726241
C          0.1384654215        0.8339998018       -1.1669972034
H         -0.4473856358       -1.1740718735       -1.0693769599
H         -2.8566429674       -0.8100391659       -0.6875698815
H         -2.5962077721        0.9236958761       -0.5038595757
C          0.0228673240       -1.4829164545        1.3973465503
C         -0.1908345508       -1.6824784747        2.8820184110
H          0.7227077661       -2.0589027673        3.3205314941
H         -0.9654529852       -2.4298211470        3.0225736047
H         -0.4933569885       -0.7749109657        3.3918640534
O          0.7470268833       -2.1981362610        0.7600154796
H         -1.3156340360        0.0358402659        1.4124280761
N          0.9943878289        1.4347105369       -0.3242159740
C          1.9788359814        2.3835390720       -0.8024695148
H          2.4861917363        2.8118782871        0.0516899601
H          1.4939742608        3.1734090887       -1.3584660598
H          2.7078898002        1.9077186190       -1.4481750712
H          1.0864861575        1.0644162450        0.5919928593
O          0.0633967571        1.1195944988       -2.3355639617

AD: Beta2 conformer, energy in hartrees.
RHF/AUG-CC-PVDZ=-492.929367
H         -2.3162824549        0.1797006135       -2.0557145056
C         -2.2441887988        0.0370112255       -0.9825960146
C         -0.7953639915       -0.2597849903       -0.5946720004
N         -0.6857399853       -0.4546781295        0.8430175483
C          0.1310837946        0.8190490038       -1.1662202806
H         -0.4750689404       -1.1817605931       -1.0706040286
H         -2.8854575519       -0.7926030191       -0.6868998311
H         -2.6023870439        0.9459571712       -0.4937581731
C          0.0417086815       -1.4646025053        1.3970840846
C         -0.1825339912       -1.6978293626        2.8749080762
H          0.7331921620       -2.0836422168        3.3119628317
H         -0.9627597158       -2.4512753579        2.9889429152
H         -0.4939104069       -0.7950487388        3.3988618725
O          0.8080132998       -2.1316979067        0.7572531286
H         -1.3693340337       -0.0152503210        1.4175844824
N          0.9671399250        1.4445159152       -0.3166402329
C          1.9748012375        2.3653920991       -0.8033440369
H          2.4309398457        2.8631646343        0.0490767717
H          1.5142982653        3.1102061815       -1.4452981503
H          2.7487798622        1.8516927847       -1.3738283274
H          1.0619079707        1.0679307606        0.5966527087
O          0.0786418091        1.0787792542       -2.3413254717

AD: Beta2 conformer, energy in hartrees.
B3LYP/6-31G(D)=-495.8501992
H         -2.2478017152        0.0783739987       -2.0358830270
C         -2.1512746079       -0.1025524752       -0.9637145966
C         -0.6697094562       -0.2097787250       -0.5901191534
N         -0.4765479616       -0.4005768049        0.8470144554
C          0.1249702630        0.9902241259       -1.1507665991
H         -0.2431685186       -1.1080836057       -1.0508155145
H         -2.6762201526       -1.0258799962       -0.7003200076
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H          -2.6306263406        0.7344832737       -0.4407270409
C          -0.0797044584       -1.6104943269        1.3781534971
C          -0.1803720592       -1.7166980621        2.8927234478
H           0.7295430343       -2.1873220235        3.2734936151
H          -1.0199096035       -2.3730594511        3.1476575502
H          -0.3257745752       -0.7533451393        3.3921178322
O           0.3330219028       -2.5305906712        0.6876196092
H          -0.9579788096        0.2445985809        1.4611157187
N           1.1816387467        1.3947758961       -0.3937966240
C           2.1017454116        2.4299044958       -0.8260517790
H           2.2172951889        3.1980737220       -0.0528207758
H           1.6839326128        2.8840880673       -1.7257855545
H           3.0900627802        2.0163974138       -1.0626807535
H           1.3759411478        0.8693313051        0.4467520618
O          -0.1836295406        1.5030056737       -2.2208668375

AD: Beta2 conformer, energy in hartrees.
B3LYP/6-31+G(D)=-495.8740391
H          -2.2867577195        0.1268139361       -2.0719464556
C          -2.2095635676       -0.0349594573       -0.9945957227
C          -0.7400438503       -0.2290545693       -0.6025301777
N          -0.5987661752       -0.4187760050        0.8420674797
C           0.1325645610        0.9138016130       -1.1676519748
H          -0.3570648770       -1.1489752911       -1.0583722951
H          -2.7932400446       -0.9191914632       -0.7182693953
H          -2.6405929596        0.8415812162       -0.4931307644
C          -0.0388779242       -1.5473542606        1.3977707128
C          -0.1819088289       -1.6801815817        2.9054971179
H           0.8084445598       -1.8400486281        3.3426267542
H          -0.7822642396       -2.5701662220        3.1229642752
H          -0.6492302419       -0.8129566839        3.3839026813
O           0.5534677975       -2.3866467129        0.7280396218
H          -1.1768423886        0.1604876169        1.4388988863
N           1.0925672284        1.4073429360       -0.3429633173
C           2.0669099158        2.3878037733       -0.7986406640
H           2.5365313220        2.8538945638        0.0715228425
H           1.5595029850        3.1530127535       -1.3906385834
H           2.8419819832        1.9282062800       -1.4249311019
H           1.2316445213        0.9415215619        0.5430520855
O          -0.0438680609        1.3248365552       -2.3128525986

AD: Beta2 conformer, energy in hartrees.
MP2/6-311++G(d,p)=-494.6204536
H          -2.3474240482        0.3006511707       -2.0408055354
C          -2.2808239910        0.1572449534       -0.9611378785
C          -0.8618060404       -0.2700554679       -0.5918758751
N          -0.7536687676       -0.4447940153        0.8512081789
C           0.1391760519        0.7331919270       -1.1782817282
H          -0.6214835112       -1.2273152132       -1.0662626440
H          -3.0017570042       -0.6069063986       -0.6559865660
H          -2.5352761273        1.1042037245       -0.4715258009
C           0.0688883042       -1.4129040016        1.3862621843
C          -0.1300264871       -1.6880156923        2.8639567149
H           0.8482698147       -1.7833043935        3.3377091153
H          -0.6506370203       -2.6440784291        2.9702855020
H          -0.7085929825       -0.9104752053        3.3687568736
O           0.9034825368       -1.9974115802        0.7088489073
H          -1.5214345173       -0.1144752015        1.4199636578
N           0.8750666149        1.4455842833       -0.2857015088
C           1.9446398317        2.3130469415       -0.7521018470
H           2.3009468926        2.9143352553        0.0857323024
H           1.5577561356        2.9715236635       -1.5310785702
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H          2.7761863511        1.7365897442       -1.1700272659
H          0.8736814773        1.1210388385        0.6694789495
O          0.2089791623        0.8896151562       -2.3933134236

AD: Beta2 conformer, energy in hartrees.
MP2/6-31G(d)=-494.3056665
H         -2.1707711972       -0.0701145037       -2.0371209262
C         -2.0571146182       -0.2061437257       -0.9610345413
C         -0.5786172655       -0.2259077887       -0.5925509476
N         -0.3688096043       -0.3877992099        0.8415366598
C          0.1402525151        1.0115539915       -1.1376644899
H         -0.1035163452       -1.1014804059       -1.0498308882
H         -2.5256943494       -1.1462325688       -0.6588154093
H         -2.5667525340        0.6234998627       -0.4604482646
C         -0.1158334104       -1.6337603608        1.3817768668
C         -0.2526688456       -1.7089027626        2.8879303270
H          0.3625089152       -2.5318334832        3.2516732746
H         -1.2952804940       -1.9150862912        3.1495718371
H          0.0490029438       -0.7784316901        3.3760456602
O          0.1993374977       -2.6024770567        0.6923776440
H         -0.8329757036        0.2867921476        1.4420770619
N          1.1903243784        1.4454799116       -0.3895831165
C          2.0625158164        2.5075630517       -0.8531456007
H          2.3625495890        3.1369413093       -0.0123642871
H          1.5016113765        3.1017775047       -1.5738975354
H          2.9580666027        2.1128022156       -1.3443279477
H          1.4567757287        0.8778562675        0.4044609270
O         -0.2165041355        1.5441433431       -2.1926986429

AD: Beta2 conformer, energy in hartrees.
MP2/6-31+G(d)=-494.3410836
H         -2.3505209156        0.2730971143       -2.0580426438
C         -2.2888354237        0.1261031921       -0.9780206380
C         -0.8672540502       -0.2810162802       -0.6023561480
N         -0.7686365991       -0.4630758595        0.8420617753
C          0.1258180733        0.7365760245       -1.1712643951
H         -0.6113291003       -1.2363706057       -1.0756228845
H         -2.9996889273       -0.6516453941       -0.6814338175
H         -2.5634376303        1.0680975852       -0.4885342088
C          0.0794756734       -1.3949389826        1.3926767247
C         -0.1212384136       -1.6788262948        2.8651415675
H          0.8486567203       -1.9014136375        3.3131127554
H         -0.7567136684       -2.5638412967        2.9736846611
H         -0.5889895347       -0.8451028356        3.3969907703
O          0.9450339720       -1.9626042303        0.7167676604
H         -1.5328034511       -0.1143026099        1.4128481640
N          0.8866003135        1.4195173811       -0.2793265518
C          1.9485091533        2.3011300855       -0.7412235020
H          2.3136848275        2.8811617502        0.1079660391
H          1.5475537682        2.9766341844       -1.4981902684
H          2.7739902540        1.7340487656       -1.1839110004
H          0.9070184299        1.0721363729        0.6716456782
O          0.1709639220        0.9323846663       -2.3941903434

AD: Beta2 conformer, energy in hartrees.
MP2/6-31++G(d,p)=-494.4394365
H         -2.3419980029        0.2590271704       -2.0509438878
C         -2.2800986181        0.1144017820       -0.9750580007
C         -0.8538678517       -0.2718145333       -0.5986903026
N         -0.7501868769       -0.4522966582        0.8442982403
C          0.1265482507        0.7564083178       -1.1707522600
H         -0.5848575504       -1.2215888874       -1.0665098477
```

```
H          -2.9760192552       -0.6698305505       -0.6769397935
H          -2.5651799896        1.0490232094       -0.4868509304
C           0.0672854310       -1.4138745841        1.3912280567
C          -0.1303936019       -1.6807471279        2.8669188039
H           0.8407234277       -1.8614591635        3.3206947957
H          -0.7308588465       -2.5834993642        2.9806502591
H          -0.6285157808       -0.8597650961        3.3812301656
O           0.9053158086       -2.0172961567        0.7130733941
H          -1.4926267961       -0.0770497296        1.4179407377
N           0.9064406405        1.4214289469       -0.2811261671
C           1.9603327133        2.3074386287       -0.7480489809
H           2.3319327060        2.8817623963        0.0968793337
H           1.5501711428        2.9827609327       -1.4944519704
H           2.7801805169        1.7480264091       -1.2007022275
H           0.9345677920        1.0657621011        0.6615998968
O           0.1509174853        0.9712998632       -2.3903715118

AD: Beta2 conformer, energy in hartrees.
RHF/CC-PVDZ=-492.9003160
H          -2.1328590101       -0.1282097058       -2.0766360806
C          -2.0358232094       -0.2535831966       -1.0011173700
C          -0.5653940732       -0.2310618766       -0.5948592281
N          -0.3798266990       -0.4074487036        0.8365499076
C           0.1378879720        1.0239043664       -1.1189577264
H          -0.0557052794       -1.0712584725       -1.0643282864
H          -2.4825352049       -1.2047716221       -0.7081349082
H          -2.5885353320        0.5566950212       -0.5183819016
C          -0.1211260178       -1.6353542032        1.3834088094
C          -0.2665217877       -1.7037452347        2.8864530224
H           0.2345103986       -2.5969478027        3.2490294938
H          -1.3269761502       -1.7659103400        3.1419105511
H           0.1493491692       -0.8194835035        3.3712670954
O           0.2045919445       -2.5797903283        0.7264896273
H          -0.8283115203        0.2612229287        1.4295212945
N           1.1920125258        1.4627705345       -0.3983554249
C           2.0551021190        2.5157973487       -0.8868377000
H           2.5860847180        2.9608500998       -0.0459541249
H           1.4514654957        3.2788312896       -1.3701289164
H           2.7865865938        2.1480235884       -1.6111572057
H           1.5150381818        0.8803115684        0.3424204701
O          -0.2318623027        1.5569966921       -2.1284055902

AD: Beta2 conformer, energy in hartrees.
DF-LMP2/AVTZ  ENERGY=-494.93853313
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0871646839
C           0.0000000000        1.4396861041        1.5915622969
H           0.8814467681       -0.5304379744        1.4464133192
H          -0.8943672778       -0.5251364000        1.4290219724
N          -0.0463063917        1.4546128745        3.0465635736
C          -1.1382991385        2.2127429457        0.9138489650
H           0.9150188071        1.9488160971        1.2823976784
C           0.5503048366        2.4518053703        3.7752685307
H          -0.2760444962        0.5948919209        3.5188565630
N          -2.0910777617        2.7283810854        1.7247153374
O          -1.1693495327        2.3108112329       -0.3100112936
C           0.6379911401        2.2078593513        5.2665357535
O           0.9761164857        3.4722944420        3.2480008958
C          -3.1368545540        3.5752848974        1.1793086499
H          -1.9057156465        2.7324700406        2.7130587583
H           0.3408798595        3.1152019117        5.7870739036
H           1.6778860076        2.0038363819        5.5201763365
```

```
H          0.0220518449        1.3746779984        5.6007943526
H         -3.8896711828        3.7424797490        1.9453050086
H         -3.5923191663        3.0788769218        0.3259214843
H         -2.7385960681        4.5338006679        0.8445555598
```

4 Total energies (hartrees) for AD at various levels of theory

theory[a]	C7ax	C5	C7ax	β_2
DF-MP2/AVTZ	-494.9676076	-494.9652806	-494.9639514	-494.9627580
DF-MP2/AVQZ	-495.1078194	-495.1056458	-495.1040547	-495.1029070
DF-MP2//CBS	-495.1879990	-495.1859007	-495.1841826	-495.1830224
DF-LMP2/AVTZ	-494.9430884	-494.9411504	-494.9392434	-494.9385331
DF-LMP2/AVQZ[b]	-495.0955857	-495.0936058	-495.0917027	-495.0908265
DF-LMP2/CBS	-495.1847304	-495.1826834	-495.1808472	-495.1798040
DF-LMP4/AVTZ	-495.0891102	-495.0872571	-495.0852330	-495.0848825
DF-LCCSD(T0)/AVTZ	-495.0887607	-495.0869369	-495.0849743	-495.0844500
DF-LCCSD(T0)/AVQZ[b]	-495.2284865	-495.2265977	-495.2246432	-495.2239155
DF-LCCSD(T0)/CBS	-495.3083114	-495.3063387	-495.3044541	-495.3035322

[a] Geometry at DF-LMP2/AVTZ. [b] Value at THRBP = 0.992.

5 Geometries and total energies at DF-LCCSD(T)/AVTZ//DF-LMP2/AVTZ

5.1 Confomers for GDA

```
GDA: C5 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27072241, DF-LCCSD(T0)=-377.35777466
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0933682893
N          0.0000000000        1.3437284710        1.6062800349
C          1.2413486414       -0.7148441379        1.6085523800
H         -0.8963520850       -0.5389736608        1.4119859176
C         -0.9943901759        2.2093110025        1.3052393082
H          0.7754372594        1.6054527939        2.1985519684
N          1.3648377532       -2.0017056179        1.1957451657
O          2.0573181384       -0.1642145090        2.3367435995
H         -0.8579197627        3.1969067874        1.7688754795
O         -1.9510195173        1.9324132809        0.5920790811
H          2.1634821601       -2.5316159939        1.5004782917
H          0.6838712167       -2.4343597459        0.5982841172

GDA: C7 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27153945, DF-LCCSD(T0)=-377.35848026
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0860288442
N          0.0000000000        1.3768351924        1.5585035998
C          1.2335985773       -0.7812544518        1.5477233312
H         -0.9064258585       -0.4817736229        1.4547483222
C         -0.4290119242        1.7148994758        2.7954242400
H          0.3861188105        2.0986666189        0.9727078039
N          1.2682076135       -1.0203243975        2.8820251789
O          2.0951174507       -1.1489942002        0.7583231644
H         -0.3877485477        2.7958354852        2.9863387771
O         -0.8323155696        0.9095963941        3.6298780484
H          2.0836213362       -1.4683557891        3.2654230970
H          0.5604310319       -0.6300758171        3.4884322606
```

5.2 Confomers for GD

```
GD: C5 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71501260, DF-LCCSD(T0)=-455.84127813
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0934500160
N          0.0000000000        1.3442093264        1.6048513217
C          1.2423723865       -0.7121562667        1.6135125610
H         -0.8982255944       -0.5367826554        1.4107441642
C         -1.0008762253        2.2080737854        1.2962629582
H          0.7776132412        1.5975774810        2.1964551500
N          1.3785625122       -1.9963937900        1.2116376941
O          2.0601274281       -0.1576753082        2.3452634759
C         -0.8849190467        3.5914034338        1.8963189633
O         -1.9395728146        1.8788074858        0.5732532681
C          2.5177318794       -2.7944044356        1.6328811587
H          0.6784414086       -2.3978012121        0.6122766708
H         -1.7710336662        3.7820830831        2.4990051651
H          0.0045771884        3.7161019418        2.5106776973
H         -0.8710383769        4.3191299246        1.0869867990
```

```
H          2.4260469072       -3.7859932018        1.1985409814
H          3.4483249866       -2.3381178112        1.2995303135
H          2.5465707701       -2.8761472370        2.7181361490

GD: C7 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71667790, DF-LCCSD(T0)=-455.84273342
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0866179421
N          0.0000000000        1.3778966017        1.5563612842
C          1.2357722658       -0.7768153547        1.5470504106
H         -0.9074212633       -0.4790015016        1.4555557858
C         -0.4295243552        1.7112221864        2.8006391421
H          0.4031990956        2.0900050950        0.9717647839
N          1.2585403452       -1.0539055807        2.8697924530
O          2.1252400292       -1.1077755682        0.7642779683
C         -0.3913471547        3.1807250245        3.1468253255
O         -0.8349249097        0.8630607121        3.5990947295
C          2.4072649271       -1.7080232670        3.4685525071
H          0.5208159923       -0.6642554968        3.4429890183
H          0.2220265976        3.3113652844        4.0363809454
H         -0.0007478476        3.8007729980        2.3424618033
H         -1.4025197139        3.5019270743        3.3905343337
H          2.1947865227       -1.8898739063        4.5185617422
H          2.6009930686       -2.6558331451        2.9696330129
H          3.3023276640       -1.0914427088        3.3811908436
```

5.3 Confomers for ADA

```
ADA: Beta2 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49356355, DF-LCCSD(T0)=-416.60035441
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0869141613
C          0.0000000000        1.4391357208        1.5925519561
H          0.8812854746       -0.5286709506        1.4478748951
H         -0.8941932506       -0.5252483190        1.4284553130
N         -0.0402108508        1.4554497422        3.0473096690
C         -1.1376682640        2.2162050397        0.9158736921
H          0.9159848116        1.9474503737        1.2846467952
C          0.5876079273        2.4169443189        3.7832606760
H         -0.3344687946        0.6198408957        3.5287747319
N         -2.0623527345        2.7805171512        1.7373859222
O         -1.1972283467        2.2701516104       -0.3047343361
H          0.5844198950        2.1941743726        4.8614938480
O          1.0839507207        3.4289722616        3.3144229923
H         -2.7291719664        3.4031001872        1.3109082076
H         -1.8671473661        2.8797334795        2.7176128599

ADA: C5 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49662246, DF-LCCSD(T0)=-416.60322701
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0900567719
C          0.0000000000        1.4302684677        1.6439015791
H          0.8930595889       -0.5133816699        1.4407581230
H         -0.8835548943       -0.5328122900        1.4410152950
N          0.0562969715        1.4421562140        3.0873739363
C         -1.2760158831        2.1627606762        1.2375312430
H          0.8744844921        1.9628018375        1.2597844659
C          1.2175622602        1.2461116411        3.7541718541
H         -0.7909710480        1.7006966122        3.5741717880
N         -1.3383164008        2.5241642921       -0.0695132157
```

```
O         -2.1895931249        2.3658754756        2.0289781225
H          1.1010299697        1.3248426216        4.8449216903
O          2.2913249276        1.0031991628        3.2156223348
H         -2.1608142548        3.0023093696       -0.3968044701
H         -0.5510887908        2.4228653405       -0.6840110331

ADA: C7ax conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49451609, DF-LCCSD(T0)=-416.60114442
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0895504991
C          0.0000000000        1.4470335936        1.5863886896
H          0.8953336467       -0.5122541025        1.4402638314
H         -0.8744833770       -0.5386491042        1.4453800736
N          0.0778770030        1.5361573883        3.0481524155
C         -1.1648709386        2.2378824457        0.9691474025
H          0.8895888247        1.9506118942        1.2123791922
C         -0.7367233703        0.9333303185        3.9433047468
H          0.8192816177        2.0973823933        3.4353744469
N         -2.3899971425        1.9846999471        1.4848353449
O         -0.9579469459        3.0126610094        0.0410994852
H         -0.4163502870        1.1067643071        4.9808684799
O         -1.7320487211        0.2667133707        3.6710480327
H         -3.1793376135        2.4524179156        1.0713589729
H         -2.5147149795        1.2969860917        2.2165962312

ADA: C7eq conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49802725, DF-LCCSD(T0)=-416.60458118
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0877269610
C          0.0000000000        1.4250166231        1.6079078907
H          0.8827582507       -0.5288471304        1.4447992679
H         -0.8992118000       -0.5226735951        1.4119839280
N          0.0174310734        1.4212647263        3.0692984079
C         -1.2305406723        2.2038577469        1.1055877033
H          0.8989518785        1.9578745826        1.2911093012
C          0.5162112477        2.4417304854        3.8027254774
H         -0.3958726174        0.6395283710        3.5538991836
N         -1.1210654898        3.5482101014        1.2568206340
O         -2.2043323699        1.6442970988        0.6176087025
H          0.4795233633        2.2524460207        4.8844251163
O          0.9738143254        3.4787204112        3.3289397057
H         -1.9328761149        4.1104839375        1.0602096551
H         -0.3608769149        3.9305306063        1.8035100096
```

5.4 Confomers for AD

```
AD: Beta2 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93853313, DF-LCCSD(T0)=-495.08444997
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0871646839
C          0.0000000000        1.4396861041        1.5915622969
H          0.8814467681       -0.5304379744        1.4464133192
H         -0.8943672778       -0.5251364000        1.4290219724
N         -0.0463063917        1.4546128745        3.0465635736
C         -1.1382991385        2.2127429457        0.9138489650
H          0.9150188071        1.9488160971        1.2823976784
C          0.5503048366        2.4518053703        3.7752685307
H         -0.2760444962        0.5948919209        3.5188565630
N         -2.0910777617        2.7283810854        1.7247153374
O         -1.1693495327        2.3108112329       -0.3100112936
```

```
C          0.6379911401        2.2078593513        5.2665357535
O          0.9761164857        3.4722944420        3.2480008958
C         -3.1368545540        3.5752848974        1.1793086499
H         -1.9057156465        2.7324700406        2.7130587583
H          0.3408798595        3.1152019117        5.7870739036
H          1.6778860076        2.0038363819        5.5201763365
H          0.0220518449        1.3746779984        5.6007943526
H         -3.8896711828        3.7424797490        1.9453050086
H         -3.5923191663        3.0788769218        0.3259214843
H         -2.7385960681        4.5338006679        0.8445555598

AD: C5 conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94115043, DF-LCCSD(T0)=-495.08693686
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904667840
C          0.0000000000        1.4304165522        1.6432832840
H          0.8932255758       -0.5133877736        1.4414499052
H         -0.8842058518       -0.5320060447        1.4416983170
N          0.0560403240        1.4427288083        3.0868331890
C         -1.2789180434        2.1587384097        1.2387221597
H          0.8760997454        1.9614375535        1.2614530455
C          1.2274434805        1.2637078113        3.7519877490
H         -0.8033035037        1.6703948965        3.5657714777
N         -1.3232951823        2.5878877109       -0.0433146973
O         -2.2215677776        2.3041298913        2.0165223481
C          1.1425317615        1.3385772770        5.2604189917
O          2.2869067149        1.0503325263        3.1640288990
C         -2.5057728991        3.2490232149       -0.5693023679
H         -0.5017372400        2.4998434107       -0.6155990774
H          1.8264694705        2.1112706146        5.6067621380
H          1.4785116009        0.3888206442        5.6730145676
H          0.1385377072        1.5538371413        5.6208352868
H         -2.6908001031        4.1868956038       -0.0472024694
H         -3.3786259823        2.6110588698       -0.4445668127
H         -2.3517014663        3.4477765366       -1.6263218355

AD: C7ax conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93924342, DF-LCCSD(T0)=-495.08497434
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0897714023
C          0.0000000000        1.4473339233        1.5854467615
H          0.8956144252       -0.5131530681        1.4395725413
H         -0.8747518766       -0.5376995964        1.4460216906
N          0.0847204433        1.5421706834        3.0475205886
C         -1.1563235028        2.2453098540        0.9619099786
H          0.8923841455        1.9465561891        1.2107259657
C         -0.7363143636        0.9447493023        3.9480269944
H          0.8362291275        2.0982989914        3.4188561757
N         -2.3854052013        2.0066677543        1.4620812358
O         -0.9406568677        3.0221169197        0.0305223284
C         -0.3543221234        1.1215890042        5.4008025512
O         -1.7347377777        0.2946670097        3.6251666262
C         -3.5469152359        2.6726471146        0.9023815420
H         -2.4768730548        1.3162334582        2.1990221521
H         -1.2087158113        1.5330912120        5.9344610505
H          0.5104156033        1.7657533500        5.5467703790
H         -0.1434511790        0.1387037320        5.8194701427
H         -4.4227884338        2.3793758404        1.4749382347
H         -3.6880283503        2.3975142954       -0.1427754679
H         -3.4268800352        3.7540046856        0.9518794577

AD: C7eq conformer, Basis set = Aug-cc-pVTZ, energy in hartrees.
```

```
DF-LMP2=-494.94308840, DF-LCCSD(T0)=-495.08876070
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0879380552
C          0.0000000000        1.4254112884        1.6089100163
H          0.8824753274       -0.5296946564        1.4449710329
H         -0.8997799558       -0.5223716816        1.4114022501
N          0.0195554400        1.4189104054        3.0700814611
C         -1.2323268426        2.2006144286        1.1085506870
H          0.8993448882        1.9573975694        1.2930295655
C          0.5192009414        2.4481754486        3.8010318192
H         -0.4104695365        0.6425646516        3.5468148691
N         -1.1200012546        3.5431544158        1.2292282143
O         -2.2259579928        1.6374596673        0.6528346311
C          0.4928149873        2.2718798967        5.3012988088
O          0.9764419866        3.4661940904        3.2743236170
C         -2.2465410442        4.4065938515        0.9249711794
H         -0.3291966031        3.8947665102        1.7557689528
H         -0.0706035499        3.0950518703        5.7368367685
H          1.5142888323        2.3356887834        5.6722768975
H          0.0541568573        1.3264975444        5.6143310979
H         -3.0692548225        4.2523172574        1.6246388793
H         -2.6121365882        4.1946711372       -0.0775316742
H         -1.9165604364        5.4406558153        0.9776418552
```

6 Torsional profiles at DF-LCCSD(T0)/AVTZ//DF-LMP2/AVTZ

6.1 ϕ profile for GDA

```
GDA: phi = +-000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.25886319, DF-LCCSD(T0)=-377.34573880
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0905820361
N          0.0000000000        1.4040848481        1.5333795283
C          1.0506033517       -1.0601246059        1.4585312155
H         -0.9440932853       -0.4455054642        1.4053955266
C          0.7962203982        2.1756786974        2.3089444823
H         -0.7839199976        1.9187935829        1.1612082445
N          2.1039086108       -0.7477355831        2.2275296033
O          0.8413752782       -2.1739863724        0.9865314476
H          0.4029176076        3.2012612597        2.3615230874
O          1.8227782329        1.8647797965        2.9045167161
H          2.7483316004       -1.4932126667        2.4344300266
H          2.2175504375        0.1874005607        2.6126716655

GDA: phi = +-015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.25960077, DF-LCCSD(T0)=-377.34651530
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0916407515
N          0.0000000000        1.3947520599        1.5591585876
C          1.0437901561       -1.0642795361        1.4668523641
H         -0.9462335392       -0.4392013931        1.4046696418
C          0.9090683618        2.2024635498        2.1529302397
H         -0.9050030909        1.8319402669        1.4744944348
N          2.0904734892       -0.7517303224        2.2497209402
O          0.8179875614       -2.1872565165        1.0268692393
H          0.4651349742        3.1828243156        2.3791766928
O          2.0822473403        1.9632094095        2.4200885315
H          2.7605933280       -1.4872563767        2.4073955591
```

```
H          2.3231941038        0.2210857672        2.4342212026

GDA: phi = +-030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26261050, DF-LCCSD(T0)=-377.35025819
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0920107488
N          0.0000000000        1.3669876817        1.5916591025
C          1.1815411390       -0.8196709673        1.6257724144
H         -0.9109694146       -0.4906223909        1.4303305525
C          1.1720984874        1.9960654519        1.8984139947
H         -0.7909630017        1.6438991945        2.1512174884
N          1.9226200677       -1.4545334623        0.6684983100
O          1.3482585872       -0.9764768098        2.8239406599
H          1.0271036346        2.8920083113        2.5189676581
O          2.2640308658        1.6401909864        1.4848297308
H          2.7674517372       -1.8886514884        1.0088208896
H          1.9866556377       -1.0240426242       -0.2388884558

GDA: phi = +-045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26588886, DF-LCCSD(T0)=-377.35352737
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0908612350
N          0.0000000000        1.3653926375        1.5801161207
C          1.1937809330       -0.7982212646        1.6296006865
H         -0.9103752630       -0.4907376811        1.4309204708
C          1.1723156711        2.0628694449        1.5662401519
H         -0.6380944395        1.5934423182        2.3255408339
N          1.8261644150       -1.5801394090        0.7047807944
O          1.4700792078       -0.7973469823        2.8179136229
H          1.1368614612        2.9863347948        2.1608369971
O          2.1503352179        1.7194035145        0.9198307995
H          2.6774365834       -2.0172567256        1.0237431232
H          1.8174301327       -1.2775396119       -0.2548381470

GDA: phi = +-060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26857142, DF-LCCSD(T0)=-377.35563422
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0924627431
N          0.0000000000        1.3877265022        1.5525525211
C          1.1605055753       -0.8785372279        1.5837165133
H         -0.9150034029       -0.4665088963        1.4432216839
C          0.9842164605        2.2878548822        1.3139825094
H         -0.5974239053        1.6014912538        2.3359079244
N          2.3885979953       -0.5556963902        1.1158777675
O          0.9383333500       -1.8411931564        2.3114356577
H          0.8524001164        3.2151584338        1.8888892333
O          1.9013527228        2.1411552944        0.5123567600
H          3.1691048536       -1.0782599674        1.4788326109
H          2.5351717535        0.3320645105        0.6532735720

GDA: phi = +-075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27116563, DF-LCCSD(T0)=-377.35812506
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0911170846
N          0.0000000000        1.3859771214        1.5406905393
C          1.1918456957       -0.8151605645        1.6072073481
H         -0.9029218244       -0.4821317664        1.4531327305
C          0.8297698445        2.3247438289        1.0294475476
H         -0.4937140309        1.6163740860        2.3878247169
N          2.3917122203       -0.4515707786        1.0933238837
O          1.0363151939       -1.7275852091        2.4107082268
H          0.7298377918        3.2997490976        1.5257865361
```

```
O          1.6003797188        2.1367716363        0.0926553896
H          3.2148453798       -0.9090299892        1.4484596241
H          2.4674287594        0.3666739189        0.5049231914

GDA: phi = +-090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27123425, DF-LCCSD(T0)=-377.35821098
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0901434112
N          0.0000000000        1.3846313770        1.5368479861
C          1.2131518908       -0.7645035528        1.6227572382
H         -0.8926058221       -0.4954292210        1.4616641489
C          0.6008992118        2.3612556409        0.8190705979
H         -0.4872674486        1.6345635426        2.3812776916
N          2.3865793058       -0.3737186864        1.0630856845
O          1.1106548765       -1.6373813464        2.4750057259
H          0.4455193742        3.3652424552        1.2366769241
O          1.2638084536        2.1580523729       -0.1938155145
H          3.2425674302       -0.7644203628        1.4197263255
H          2.4089861172        0.4032830475        0.4183416595

GDA: phi = +-105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26914820, DF-LCCSD(T0)=-377.35627772
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0893073986
N          0.0000000000        1.3867423898        1.5278732021
C          1.2223541282       -0.7334479210        1.6346569398
H         -0.8872770342       -0.5042365997        1.4641302098
C          0.3241498135        2.3933613545        0.6782242154
H         -0.4165182646        1.6219734095        2.4137249049
N          2.3800843337       -0.3797199725        1.0142814460
O          1.1523792186       -1.5436761699        2.5484317497
H          0.1332971862        3.3907182295        1.0979042936
O          0.8117072149        2.2213578017       -0.4327488578
H          3.2505504582       -0.7203804002        1.3868655077
H          2.3866703360        0.3593647635        0.3289610520

GDA: phi = +-120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26921066, DF-LCCSD(T0)=-377.35648032
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0906981456
N          0.0000000000        1.3714885330        1.5358270013
C          1.2190426535       -0.7300480783        1.6468408279
H         -0.8950945187       -0.5289441091        1.4282157819
C          0.0357819035        2.3952785857        0.6364181954
H          0.4209639066        1.5367594666        2.4396658082
N          1.4758627049       -1.9321702299        1.0660697663
O          1.8678561686       -0.2844062940        2.5835718514
H          0.2375162750        3.3640890400        1.1152495997
O         -0.1624916883        2.2799483700       -0.5640865814
H          2.2872856320       -2.4431198181        1.3719005808
H          1.0334263756       -2.1972718706        0.2042781739

GDA: phi = +-135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26978839, DF-LCCSD(T0)=-377.35695676
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0915730618
N          0.0000000000        1.3653610407        1.5531712654
C          1.2249150048       -0.7204512733        1.6423818287
H         -0.8933288456       -0.5380816205        1.4211420749
C         -0.2709093032        2.3913323630        0.7029090380
H          0.5679035263        1.5506000957        2.3689183961
N          1.4401792172       -1.9553566958        1.1192056375
```

```
O          1.9249599376       -0.2330363829        2.5202906604
H         -0.0606237126        3.3736115116        1.1496752747
O         -0.7230541518        2.2595516459       -0.4258696125
H          2.2465375530       -2.4714784225        1.4286536855
H          0.9254522290       -2.2846009687        0.3223667230

GDA: phi = +-150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27028082, DF-LCCSD(T0)=-377.35738736
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0923626799
N          0.0000000000        1.3573695854        1.5734018405
C          1.2321830661       -0.7148860635        1.6315135499
H         -0.8926753597       -0.5430829696        1.4156573993
C         -0.5592353044        2.3572014518        0.8473692916
H          0.6753645718        1.5713533902        2.2946415681
N          1.4040241670       -1.9777476040        1.1636914410
O          1.9839135456       -0.1939930430        2.4454384295
H         -0.3635815495        3.3514629674        1.2739420087
O         -1.2270463771        2.1867042243       -0.1640328050
H          2.2122054215       -2.4955566025        1.4647106526
H          0.8236618159       -2.3533823826        0.4355336664

GDA: phi = +-165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27060704, DF-LCCSD(T0)=-377.35767745
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0931734487
N          0.0000000000        1.3497700182        1.5915263163
C          1.2403707328       -0.7117851025        1.6158801282
H         -0.8937214370       -0.5427865155        1.4129302867
C         -0.8089622073        2.2936183136        1.0559061149
H          0.7480022136        1.5965933887        2.2246225541
N          1.3617060276       -2.0031028187        1.2159483383
O          2.0514433037       -0.1583606961        2.3473027765
H         -0.6426943468        3.2923015728        1.4847142272
O         -1.6492599542        2.0687762836        0.1939617897
H          2.1745260178       -2.5217673526        1.5021792698
H          0.7105501627       -2.4219999627        0.5767814410

GDA: phi = +-180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27072238, DF-LCCSD(T0)=-377.35777416
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0933262399
N          0.0000000000        1.3438672669        1.6060637406
C          1.2410866995       -0.7149894127        1.6087272553
H         -0.8964718879       -0.5387351985        1.4118840261
C         -0.9943607002        2.2093579062        1.3047770953
H          0.7756572000        1.6058253346        2.1978962026
N          1.3646514822       -2.0018042287        1.1957149413
O          2.0568738677       -0.1645093999        2.3372475668
H         -0.8576285998        3.1972076955        1.7677417316
O         -1.9510970487        1.9322504846        0.5918072229
H          2.1633167973       -2.5315972510        1.5005570183
H          0.6840116577       -2.4342033133        0.5977180575
```

6.2 ψ profile for GDA

```
GDA: psi = +-000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26792301, DF-LCCSD(T0)=-377.35513277
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898326506
```

```
N          0.0000000000        1.3690774626        1.5669205394
C          1.1742314195       -0.8752151665        1.5287593074
H         -0.9073795249       -0.4998123009        1.4251312797
C          0.5630006878        2.3802982210        0.8447246278
H         -0.5893717981        1.6219672976        2.3428190999
N          2.1042339864       -0.2828178555        2.3243832839
O          1.2138243358       -2.0490488818        1.1918058017
H          0.3693736400        3.3718632998        1.2814695170
O          1.2275557697        2.2143249111       -0.1650909053
H          2.9480263867       -0.8022816968        2.5040195998
H          2.1293296279        0.7186586404        2.4023263848

GDA: psi = +-015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26854810, DF-LCCSD(T0)=-377.35584732
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0918448817
N          0.0000000000        1.3732077376        1.5620235798
C          1.1617003973       -0.8986572340        1.5237649170
H         -0.9115698963       -0.4880512735        1.4268099660
C          0.7969205998        2.3356598132        1.0416522080
H         -0.6414192173        1.6394745456        2.2901748414
N          2.2595846626       -0.2799730607        2.0460777937
O          1.0430988490       -2.1116387951        1.4302048898
H          0.5994565933        3.3316353851        1.4632333077
O          1.6637465258        2.1278431640        0.2002661028
H          3.0561187747       -0.8856325584        2.1761755256
H          2.4609087118        0.6587231713        1.7348525119

GDA: psi = +-030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26994247, DF-LCCSD(T0)=-377.35712278
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0926302036
N          0.0000000000        1.3781777270        1.5520541083
C          1.1705873811       -0.8809632133        1.5405678825
H         -0.9088181813       -0.4876353719        1.4339394377
C          0.7713829103        2.3470139898        1.0103029079
H         -0.6010366183        1.6342250105        2.3177358852
N          2.3541672600       -0.2408246108        1.7512916231
O          1.0001271204       -2.0802667889        1.7110458406
H          0.5825171752        3.3391604281        1.4437236881
O          1.6062288162        2.1533190671        0.1319503020
H          3.1480806665       -0.8443087079        1.9015021043
H          2.5169404981        0.6310388839        1.2655649687

GDA: psi = +-045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27097407, DF-LCCSD(T0)=-377.35802453
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0923360443
N          0.0000000000        1.3819453441        1.5440363238
C          1.1838145165       -0.8492412003        1.5669428496
H         -0.9039193745       -0.4885308283        1.4444341118
C          0.7337141682        2.3528832545        0.9564068861
H         -0.5527176540        1.6317416823        2.3473670820
N          2.3987847438       -0.2501211038        1.4651515048
O          1.0085419133       -1.9775571132        2.0084207867
H          0.5662036811        3.3452631197        1.3972160719
O          1.5124259068        2.1628319397        0.0265072660
H          3.2049496164       -0.8208508624        1.6621188861
H          2.5014780265        0.5696134131        0.8821615346

GDA: psi = +-060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27145522, DF-LCCSD(T0)=-377.35840669
```

```
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0913926481
N          0.0000000000        1.3839600065        1.5402077384
C          1.1967926000       -0.8114641229        1.5980724725
H         -0.8992210921       -0.4893586980        1.4539205646
C          0.7147685752        2.3502184259        0.9213348371
H         -0.5197643265        1.6324907648        2.3656435168
N          2.4022829494       -0.3266180278        1.2117171536
O          1.0455557123       -1.8091967944        2.2924293707
H          0.5705042421        3.3445752559        1.3654743167
O          1.4509604035        2.1547029691       -0.0416098031
H          3.2294400233       -0.8254950355        1.4933154365
H          2.4611939162        0.4644821379        0.5860287483

GDA: psi = +-075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27147493, DF-LCCSD(T0)=-377.35844693
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0901937591
N          0.0000000000        1.3843332580        1.5398595972
C          1.2077719021       -0.7735307395        1.6261674665
H         -0.8961089173       -0.4899565630        1.4598862554
C          0.7259988321        2.3386802204        0.9135502413
H         -0.4866473825        1.6295338094        2.3862567054
N          2.3753093489       -0.4729007039        1.0019555638
O          1.0999399901       -1.5900829531        2.5326189979
H          0.6118416109        3.3338428378        1.3643793255
O          1.4385590733        2.1317225401       -0.0644459065
H          3.2241261152       -0.8601246995        1.3804691574
H          2.4157556614        0.3153936871        0.3707138984

GDA: psi = +-090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27073039, DF-LCCSD(T0)=-377.35784835
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0888776466
N          0.0000000000        1.3832907704        1.5397968542
C          1.2105965021       -0.7503023503        1.6470803923
H         -0.8964565178       -0.4894863853        1.4599029978
C          0.7703909129        2.3107344708        0.9211720539
H         -0.4193379952        1.6159199615        2.4251649878
N          2.3124044544       -0.6963163135        0.8495420332
O          1.1577854059       -1.3530157490        2.7113779919
H          0.7064851756        3.3053223021        1.3831468954
O          1.4573999447        2.0818306958       -0.0692733059
H          3.1752077185       -1.0400490795        1.2414685166
H          2.3592410084        0.0332969005        0.1519413788

GDA: psi = +-105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26945411, DF-LCCSD(T0)=-377.35675369
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0881240500
N          0.0000000000        1.3798829667        1.5421223243
C          1.2043823856       -0.7499907710        1.6592317920
H         -0.8998464105       -0.4886245677        1.4543411054
C          0.8169423346        2.2829591772        0.9427055370
H         -0.3871654714        1.6028001434        2.4445124712
N          2.2054888430       -0.9799542511        0.7632920450
O          1.2233259096       -1.1267942793        2.8232882023
H          0.7876203364        3.2749296958        1.4139613092
O          1.5044442388        2.0337728578       -0.0410724046
H          3.0709521192       -1.3329578151        1.1425028907
H          2.2677810795       -0.3631406864       -0.0330095084
```

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GDA: psi = +-120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26847725, DF-LCCSD(T0)=-377.35590564
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0878465582
N          0.0000000000        1.3768398808        1.5426605140
C          1.1954994758       -0.7604769592        1.6634642464
H         -0.9044463825       -0.4878352575        1.4466891827
C          0.8465145292        2.2656469581        0.9582910447
H         -0.3443932793        1.5829331156        2.4663348441
N          2.0516555986       -1.2782000460        0.7381808993
O          1.3188829321       -0.9158276213        2.8704758901
H          0.8422941294        3.2513986401        1.4435763978
O          1.5257422421        2.0121553745       -0.0284537664
H          2.9087281759       -1.6721817835        1.0950348380
H          2.0912269608       -0.8403050341       -0.1680543276

GDA: psi = +-135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26816587, DF-LCCSD(T0)=-377.35567228
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0879367044
N          0.0000000000        1.3737420258        1.5415066557
C          1.1931172666       -0.7691818413        1.6582484650
H         -0.9071830297       -0.4901060770        1.4400987937
C          0.8380437608        2.2654446207        0.9436505227
H         -0.2720949937        1.5594485777        2.4936226545
N          1.8609008019       -1.5503898467        0.7636799689
O          1.4661107333       -0.7152045820        2.8486627615
H          0.8616046050        3.2399132460        1.4512702285
O          1.4781033080        2.0281526603       -0.0711873624
H          2.7053284055       -1.9922185964        1.0922530742
H          1.8059268991       -1.3286951996       -0.2158422584

GDA: psi = +-150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.26948311, DF-LCCSD(T0)=-377.35664514
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0953189927
N          0.0000000000        1.3416651376        1.6243008707
C          1.2603067520       -0.7009875838        1.5792368977
H         -0.9005783322       -0.5225003110        1.4198249462
C         -1.0646611661        2.1608173571        1.4476203126
H          0.8882429628        1.7074735965        1.9366634504
N          1.1487417152       -2.0446720140        1.7394525554
O          2.2889974415       -0.0804909607        1.8163027776
H         -0.8947762517        3.1728113163        1.8433094543
O         -2.1164599182        1.8163560705        0.9245025579
H          1.9797059402       -2.5722240545        1.9500997250
H          0.3073246490       -2.5341910350        1.4932118987

GDA: psi = +-165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27040036, DF-LCCSD(T0)=-377.35751720
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0947386513
N          0.0000000000        1.3428127744        1.6135394686
C          1.2511180862       -0.7093465163        1.5918413301
H         -0.8967732249       -0.5343696338        1.4145934646
C         -0.9902501040        2.2109604044        1.3011021009
H          0.8450134626        1.6509110987        2.0738303463
N          1.2321930525       -2.0607768787        1.4529267205
O          2.1892012201       -0.1007978166        2.0902755246
H         -0.8274718754        3.2148093102        1.7192859351
O         -1.9756837695        1.9158461863        0.6366510246
H          2.0766364338       -2.5705984237        1.6522117355
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H          0.4886314264       -2.5243866294        0.9619382194

GDA: psi = +-180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-377.27072239, DF-LCCSD(T0)=-377.35777414
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0933270356
N          0.0000000000        1.3438056020        1.6061888174
C          1.2413221159       -0.7148629375        1.6084343237
H         -0.8963374615       -0.5388991849        1.4119587906
C         -0.9944395402        2.2092901344        1.3051406017
H          0.7755207953        1.6055374201        2.1983107855
N          1.3647789268       -2.0017586450        1.1956568076
O          2.0573966423       -0.1641940112        2.3364915992
H         -0.8578533916        3.1969978774        1.7684508893
O         -1.9510689303        1.9323331278        0.5919719609
H          2.1636448674       -2.5314082033        1.5002276257
H          0.6839216027       -2.4343612922        0.5980536196
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6.3 ϕ profile for GD

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GD: phi = +-000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.70281354, DF-LCCSD(T0)=-455.82869919
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0910769381
N          0.0000000000        1.4077947952        1.5289759789
C          1.0391080978       -1.0726611380        1.4549275281
H         -0.9482200063       -0.4390195644        1.4032715004
C          0.8000333606        2.1810414495        2.3065222264
H         -0.7852589923        1.9097126610        1.1470004138
N          2.1092570370       -0.7801173116        2.2008789739
O          0.8070098538       -2.1915873460        0.9923660776
C          0.3463447026        3.6219639219        2.4335813201
O          1.8241201686        1.8126552328        2.8858799037
C          3.0664854174       -1.8226831322        2.5223783115
H          2.1975195848        0.1664930340        2.5703490694
H         -0.5919460249        3.8376749891        1.9266293647
H          0.2462750687        3.8534016228        3.4921487817
H          1.1291408117        4.2605378185        2.0278003164
H          3.8650726512       -1.3832368457        3.1139784952
H          2.5923942787       -2.6241316173        3.0882839560
H          3.4819017582       -2.2539848519        1.6126358932

GD: phi = +-015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.70447816, DF-LCCSD(T0)=-455.83141277
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0887311098
N          0.0000000000        1.3876101359        1.5505111878
C          1.2426534519       -0.7782468196        1.5310146621
H         -0.9045037325       -0.5086686876        1.4309239903
C          0.8466113642        1.8367158375        2.5369037041
H         -0.2076820649        2.0687531146        0.8376421497
N          1.0128385827       -1.8012362110        2.3993565713
O          2.3405106883       -0.5387121075        1.0442739669
C          1.1059465390        3.3264454507        2.5244203615
O          1.3285112890        1.0868877284        3.3764030712
C          2.1577999250       -2.4482649858        3.0212823485
H          0.1761519269       -1.7225679195        2.9542205553
H          1.3043753061        3.6584367156        3.5392149292
H          1.9931735675        3.5146968479        1.9185216587
H          0.2726096850        3.8894589386        2.1064354482
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H          1.8072421493       -3.2899975488        3.6130793129
H          2.8268700111       -2.8084253916        2.2446353765
H          2.7063349032       -1.7497653204        3.6553975069

GD: phi = +-030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.70839197, DF-LCCSD(T0)=-455.83529124
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0888295033
N          0.0000000000        1.3836179699        1.5463605321
C          1.2441885146       -0.7637614847        1.5531397629
H         -0.9059479351       -0.5073573139        1.4279026043
C          0.6214007611        1.7086999614        2.7294844497
H          0.0838034595        2.0782819191        0.8212185119
N          1.0017166410       -1.9347762992        2.1996296839
O          2.3685044018       -0.3709335366        1.2651509168
C          1.0261706192        3.1562454081        2.8738629069
O          0.8081157587        0.8719226515        3.6047503970
C          2.1178776907       -2.6440229200        2.8051865643
H          0.1051229379       -2.0117314400        2.6510784966
H          0.9846341709        3.4332231724        3.9232786773
H          2.0565036633        3.2554961362        2.5296153834
H          0.3958566459        3.8234327083        2.2878891590
H          1.7628780020       -3.5986612811        3.1850150643
H          2.8798446581       -2.8178930361        2.0502114028
H          2.5611186590       -2.0644356295        3.6164141689

GD: phi = +-045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71163075, DF-LCCSD(T0)=-455.83849773
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0891380085
N          0.0000000000        1.3776138413        1.5477214202
C          1.2456738782       -0.7515306177        1.5680976633
H         -0.9068386176       -0.5012634283        1.4309198173
C          0.3343519348        1.6138548360        2.8590602377
H          0.3174124613        2.0676095219        0.8856691714
N          1.0204998978       -1.9970125589        2.0603080486
O          2.3654118463       -0.2714460395        1.4315457518
C          0.7474095774        3.0277401828        3.1863527233
O          0.2842921964        0.7186750638        3.6956201966
C          2.1248334474       -2.7391804908        2.6471732847
H          0.0950441673       -2.1768688378        2.4130867601
H          0.4503662492        3.2574797468        4.2056295251
H          1.8346986722        3.0856567471        3.1217436597
H          0.3163276715        3.7545092426        2.4999044259
H          1.7884130791       -3.7471223869        2.8758593059
H          2.9416720779       -2.7857196371        1.9319447990
H          2.4892854659       -2.2573880474        3.5555058104

GD: phi = +-060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71355433, DF-LCCSD(T0)=-455.83980383
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0858649365
N          0.0000000000        1.3927461758        1.5327122473
C          1.2114471578       -0.8284838342        1.5346008156
H         -0.9176255099       -0.4718470345        1.4420564873
C          0.0135185498        1.7578175510        2.8457873298
H          0.3853545164        2.0623585927        0.8860163462
N          1.2025349243       -1.2409333495        2.8205522814
O          2.1058399748       -1.1152788926        0.7370843683
C          0.3274761772        3.2105813283        3.1187476426
O         -0.2497999959        0.9703757345        3.7557600803
C          2.3451944738       -1.9580872736        3.3575172523
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H          0.5517107773       -0.7763468259        3.4417871799
H          1.3230534675        3.2691596256        3.5581604547
H          0.2972088068        3.8291135872        2.2240829391
H         -0.3835872902        3.5876363976        3.8496960043
H          2.1245648973       -2.2420509860        4.3829169609
H          2.5308244441       -2.8523880885        2.7664822853
H          3.2476139174       -1.3456471784        3.3350851859

GD: phi = +-075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71628911, DF-LCCSD(T0)=-455.84236232
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0907421936
N          0.0000000000        1.3870940645        1.5389868971
C          1.1895165489       -0.8086234848        1.6179632298
H         -0.9046886684       -0.4791450485        1.4540736804
C          0.8428571140        2.3186158324        1.0210101838
H         -0.4868443880        1.6086440834        2.3912984671
N          2.3780219253       -0.5118968857        1.0477159350
O          1.0473536977       -1.6650979575        2.4906090494
C          0.7905211109        3.6872240873        1.6578789016
O          1.5902368722        2.0718838003        0.0716218948
C          3.5974220225       -1.1355479152        1.5282708040
H          2.4116581295        0.2974755977        0.4400473074
H          0.5821783900        4.4199844313        0.8808033169
H          0.0401882591        3.7676046041        2.4417100531
H          1.7717610720        3.9125606870        2.0724804050
H          3.7966520510       -0.8688526746        2.5668302329
H          3.5099199245       -2.2186718146        1.4697913807
H          4.4241720992       -0.8061417766        0.9048008457

GD: phi = +-090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71636661, DF-LCCSD(T0)=-455.84247062
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0899743837
N          0.0000000000        1.3848439023        1.5363479954
C          1.2091455738       -0.7649220705        1.6281129174
H         -0.8944596725       -0.4932279278        1.4616089056
C          0.6097290047        2.3602238955        0.8135869252
H         -0.5012147444        1.6301851306        2.3727597392
N          2.3814538123       -0.4051278917        1.0567168964
O          1.1103270372       -1.6168198821        2.5090817151
C          0.4354331721        3.7728552969        1.3180257947
O          1.2726797367        2.1014168690       -0.1932962887
C          3.6376011153       -0.9530656172        1.5348576501
H          2.3663122901        0.3658558386        0.4017608716
H         -0.0773933932        4.3497073014        0.5500182878
H         -0.1295398884        3.8292339695        2.2463362755
H          1.4192552327        4.2143259181        1.4635596108
H          3.8222875096       -0.6688983151        2.5712664743
H          3.6160941236       -2.0399103924        1.4815999131
H          4.4418017485       -0.5773343357        0.9081589537

GD: phi = +-105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71418425, DF-LCCSD(T0)=-455.84047184
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0877670378
N          0.0000000000        1.3701248791        1.5768763963
C          1.2536958174       -0.7327448641        1.5554546846
H         -0.9006200863       -0.4831384459        1.4639990123
C         -0.8082365600        1.7446812651        2.6081526618
H          0.4425293751        2.0814701734        1.0200997249
N          1.2199553773       -1.0695888236        2.8681676620
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O          2.2040166714       -0.9670712510        0.8135524491
C         -0.9078953178        3.2297077061        2.8662841329
O         -1.4028554307        0.9160128485        3.2969283731
C          2.3804186593       -1.6431779850        3.5245635121
H          0.4319735842       -0.7513563202        3.4136333134
H         -0.7420049720        3.4125285703        3.9254321398
H         -0.2008224924        3.8126982931        2.2792396318
H         -1.9207119624        3.5514229921        2.6267304045
H          2.0881227384       -1.9921567891        4.5113229980
H          2.7517074421       -2.4821935996        2.9403417908
H          3.1853972703       -0.9136719879        3.6224369206

GD: phi = +-120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71374116, DF-LCCSD(T0)=-455.84014077
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0933857825
N          0.0000000000        1.3455697753        1.6140249574
C          1.2485856095       -0.7378099990        1.5661509691
H         -0.9133129818       -0.4895713098        1.4328660125
C         -1.0156746290        1.7793442743        2.4227088996
H          0.9150565512        1.7531228577        1.7411700088
N          1.1896805823       -2.0877232277        1.4850925508
O          2.2522159086       -0.1369237487        1.9430342240
C         -0.7732922750        3.1078273325        3.1031009440
O         -2.0655033021        1.1586974772        2.5601383906
C          2.3246760021       -2.9090338920        1.8722300421
H          0.3076093251       -2.5223692243        1.2761244847
H         -0.9142485938        2.9765017632        4.1741700322
H          0.2192165210        3.5107306382        2.9122583005
H         -1.5221706991        3.8164375424        2.7535717338
H          2.1073209367       -3.9438836488        1.6223858737
H          3.2134129142       -2.5863221563        1.3343035883
H          2.5227379652       -2.8273003044        2.9404276164

GD: phi = +-135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71417553, DF-LCCSD(T0)=-455.84051981
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0940063410
N          0.0000000000        1.3407811276        1.6231576856
C          1.2492113108       -0.7300939290        1.5749029154
H         -0.9104003422       -0.5039567850        1.4234023223
C         -1.1319711807        1.8783631630        2.1660243890
H          0.9026736617        1.6816382189        1.9227537088
N          1.2529738760       -2.0667912511        1.3641311762
O          2.1989695447       -0.1344837462        2.0790845875
C         -0.9373260656        3.1850163061        2.9021790223
O         -2.2337427719        1.3482471164        2.0526194605
C          2.3921631870       -2.8815855932        1.7521848631
H          0.4126998831       -2.5081485640        1.0326639752
H         -1.1573816094        3.0221738519        3.9563831642
H          0.0703931251        3.5831047600        2.8023003988
H         -1.6546591707        3.9082676645        2.5205177643
H          2.2337923086       -3.8947119555        1.3929689467
H          3.3015636648       -2.4797355109        1.3105858973
H          2.5146076300       -2.8956047058        2.8346746307

GD: phi = +-150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71458350, DF-LCCSD(T0)=-455.84089363
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0924486387
N          0.0000000000        1.3584348153        1.5710018385
C          1.2338763419       -0.7109376197        1.6357515738
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H         -0.8941295099       -0.5411845981        1.4152834076
C         -0.5628879272        2.3568792051        0.8350419400
H          0.6840977803        1.5644773480        2.2851941534
N          1.4217829075       -1.9690811716        1.1748272935
O          1.9851369614       -0.1861126054        2.4552365057
C         -0.3550732050        3.7561769755        1.3698340764
O         -1.2211741160        2.1308173817       -0.1776101492
C          2.5647170797       -2.7584123283        1.6028145677
H          0.8191520695       -2.3155301345        0.4484280667
H         -1.3117292446        4.1358154261        1.7260565914
H          0.3687120715        3.7984191031        2.1813850400
H         -0.0277930864        4.3936510556        0.5514791639
H          3.4988841740       -2.3089594178        1.2678996761
H          2.5860629280       -2.8222946860        2.6886561992
H          2.4733784737       -3.7570381421        1.1846655388

GD: phi = +-165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71490352, DF-LCCSD(T0)=-455.84118540
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0935686742
N          0.0000000000        1.3405204766        1.6160890682
C          1.2430513515       -0.7179882610        1.6049520149
H         -0.9016050363       -0.5300678476        1.4118386583
C         -1.1240576550        2.1035799238        1.5750654793
H          0.8038425436        1.5986939573        2.1699716405
N          1.3698149508       -2.0030720446        1.2017890527
O          2.0732682748       -0.1638725917        2.3226513704
C         -1.0261854170        3.4535110179        2.2499217410
O         -2.1475263334        1.7208194211        1.0116727344
C          2.4974416400       -2.8136707202        1.6300061036
H          0.6369679150       -2.4154810468        0.6508150092
H         -1.7974931980        3.5137101507        3.0156289133
H         -0.0523288906        3.6350512573        2.7002282609
H         -1.2316708374        4.2252529573        1.5103696873
H          2.4520765257       -3.7703747088        1.1171041645
H          3.4314489276       -2.3141810760        1.3810747816
H          2.4737135461       -2.9784525213        2.7065681256

GD: phi = +-180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71500785, DF-LCCSD(T0)=-455.84127427
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0936690061
N          0.0000000000        1.3440092855        1.6058906176
C          1.2434343263       -0.7118191442        1.6111602708
H         -0.8989273744       -0.5355528845        1.4104893598
C         -1.0019805359        2.2072952075        1.2992924302
H          0.7913577364        1.6055740123        2.1752706431
N          1.3614133926       -2.0063287955        1.2375400895
O          2.0800899843       -0.1468377877        2.3129178206
C         -0.8828327723        3.5923182949        1.8948132831
O         -1.9474960116        1.8741701403        0.5869953340
C          2.5049599515       -2.8021874797        1.6509303510
H          0.6435868738       -2.4175043725        0.6664103588
H         -1.7443605935        3.7674827239        2.5369000449
H          0.0302179805        3.7314456719        2.4703014840
H         -0.9175786032        4.3204268078        1.0867042359
H          2.4086135842       -3.7961088835        1.2229747224
H          3.4309500329       -2.3470168095        1.3038018122
H          2.5472330493       -2.8782783043        2.7362403399
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6.4 ψ profile for GD

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GD: psi = +-000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71282864, DF-LCCSD(T0)=-455.83913865
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0890314495
N          0.0000000000        1.3697708520        1.5666637755
C          1.1751254743       -0.8718849573        1.5312491104
H         -0.9051762444       -0.4982945720        1.4351686085
C         -0.6244363499        1.7145850032        2.7377798601
H          0.2712342269        2.1043158359        0.9356797140
N          2.0992055415       -0.2809363165        2.3241283148
O          1.2540604596       -2.0322930341        1.1410840757
C         -0.7142224134        3.1983413301        3.0198546077
O         -1.0679743384        0.8695090579        3.5052573122
C          3.1867848156       -1.0553344914        2.8944826863
H          1.8749384986        0.6238852041        2.7019703936
H         -0.3611017857        3.3828495453        4.0320478831
H         -0.1442679463        3.8048357747        2.3182129365
H         -1.7620556990        3.4924854179        2.9757246247
H          2.8390504634       -1.6983643913        3.7038688963
H          3.6173583427       -1.6842925162        2.1195073596
H          3.9455097792       -0.3750675666        3.2728173183

GD: psi = +-015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71317639, DF-LCCSD(T0)=-455.83960618
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0916373214
N          0.0000000000        1.3734215039        1.5593645553
C          1.1605683194       -0.8984498046        1.5255387827
H         -0.9120120452       -0.4877588263        1.4281355689
C          0.7671314517        2.3447309506        0.9932614055
H         -0.6179253883        1.6261137962        2.3109274803
N          2.2538090396       -0.2853608069        2.0452621360
O          1.0495334034       -2.1159994275        1.4199557410
C          0.5381219005        3.7497199120        1.5022259293
O          1.5942633992        2.0867698372        0.1199452807
C          3.4388107776       -1.0801588755        2.3295679111
H          2.3857812606        0.6806276298        1.7866947867
H          0.0600194182        4.3255410888        0.7106233810
H         -0.0860027963        3.7863706851        2.3931027370
H          1.5019863002        4.2081452155        1.7109487618
H          4.1553432388       -0.4606935335        2.8625891773
H          3.1580815983       -1.9253057864        2.9523216976
H          3.8957754734       -1.4655039536        1.4169233342

GD: psi = +-030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71466211, DF-LCCSD(T0)=-455.84096324
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0925310287
N          0.0000000000        1.3786483594        1.5518461897
C          1.1625594322       -0.8892913272        1.5450119631
H         -0.9115666582       -0.4839467696        1.4334802448
C          0.7781410252        2.3480450048        1.0070691540
H         -0.6078098977        1.6266166838        2.3133986986
N          2.3460867507       -0.2662805460        1.7646148736
O          0.9843102112       -2.0936937227        1.7073292220
C          0.5646550433        3.7473903775        1.5353441555
O          1.6114497088        2.0980571197        0.1337151591
C          3.5210575822       -1.0658813789        2.0721116864
H          2.4716719942        0.6254884972        1.3028848826
H          0.1983973494        4.3678955405        0.7187554112
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H          -0.1416309306        3.7917273553        2.3620156750
H           1.5240990817        4.1499377421        1.8534085993
H           4.3423484156       -0.3972590306        2.3163826273
H           3.3088084836       -1.7037782361        2.9265416121
H           3.8065696874       -1.7042600341        1.2347080694

GD: psi = +-045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71588858, DF-LCCSD(T0)=-455.84204717
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0923110999
N           0.0000000000        1.3824119490        1.5437261549
C           1.1761625677       -0.8575772706        1.5712115135
H          -0.9068479459       -0.4848758190        1.4434822585
C           0.7436402736        2.3538964176        0.9576135880
H          -0.5644021393        1.6251118002        2.3397493051
N           2.3935337664       -0.2747977122        1.4805866273
O           0.9923730633       -1.9915674523        2.0089827515
C           0.5608565731        3.7512046985        1.5013879787
O           1.5245369127        2.1095683460        0.0346209346
C           3.5869665739       -1.0288541147        1.8214119821
H           2.4632389470        0.5622965903        0.9148424445
H           0.1943190682        4.3859824372        0.6962868272
H          -0.1315067789        3.7991191672        2.3395015796
H           1.5319298754        4.1336243807        1.8096446036
H           4.4426221844       -0.3597244592        1.7861832016
H           3.4884295986       -1.4366341159        2.8250835549
H           3.7467305720       -1.8597347783        1.1330006261

GD: psi = +-060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71653519, DF-LCCSD(T0)=-455.84259189
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0865290873
N           0.0000000000        1.3772088571        1.5571780594
C           1.2176006206       -0.8106290354        1.5398553247
H          -0.9109669435       -0.4785891699        1.4499877884
C          -0.4328661756        1.7228588229        2.7958089635
H           0.3691665202        2.0928334920        0.9548520889
N           1.3569864167       -0.9164985747        2.8792909504
O           1.9961319729       -1.3136695299        0.7310075884
C          -0.4192997774        3.1980776746        3.1186931165
O          -0.8181013605        0.8804014337        3.6104901990
C           2.4659186191       -1.6565368042        3.4518062205
H           0.6355883875       -0.5132060431        3.4638207513
H           0.1934518224        3.3531998153        4.0047160258
H          -0.0411558724        3.8124575548        2.3040861366
H          -1.4354382914        3.5053391290        3.3597653929
H           2.4037301251       -2.7147445742        3.1981108230
H           3.4117967768       -1.2740536385        3.0713682876
H           2.4381053407       -1.5426781252        4.5321313191

GD: psi = +-075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71664487, DF-LCCSD(T0)=-455.84272230
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0901022598
N           0.0000000000        1.3853444576        1.5367778739
C           1.2041891582       -0.7749898156        1.6282632146
H          -0.8982247037       -0.4876696696        1.4593898699
C           0.7250449265        2.3393535721        0.8971868951
H          -0.4795922507        1.6224120468        2.3883790538
N           2.3718407380       -0.4824316608        1.0109939712
O           1.0994947475       -1.5854479924        2.5475403900
C           0.6232205866        3.7388138920        1.4554930494
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O          1.4171983655        2.0787128457       -0.0897139476
C          3.6207400493       -1.0500210840        1.4847795065
H          2.3695649209        0.2934925308        0.3607759912
H          0.2315115621        4.3908678312        0.6767156626
H         -0.0152131066        3.8041736706        2.3342847810
H          1.6237093765        4.0857365191        1.7070092012
H          3.8827409870       -0.6706055766        2.4734352888
H          3.5305345821       -2.1321415777        1.5514616015
H          4.4081708775       -0.7959374176        0.7802782644

GD: psi = +-090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71600456, DF-LCCSD(T0)=-455.84222374
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0871669093
N          0.0000000000        1.3780033473        1.5540541056
C          1.2576629323       -0.7319940307        1.5547115824
H         -0.9032284350       -0.4813822518        1.4584950246
C         -0.3899164006        1.6748025720        2.8233483177
H          0.4631000578        2.0804355863        1.0028384935
N          1.1303423697       -1.3480083552        2.7553417473
O          2.2850390684       -0.7495237462        0.8796097555
C         -0.2994869557        3.1277681065        3.2251352931
O         -0.8094726557        0.8080118113        3.5923482746
C          2.2879801318       -1.9523975969        3.3912254157
H          0.3434879451       -1.0587892186        3.3214481415
H          0.3299979326        3.2037715112        4.1097369429
H          0.1005342029        3.7647493973        2.4389067734
H         -1.2959740745        3.4724795062        3.4956644442
H          1.9570398500       -2.5073323818        4.2649577946
H          2.7679767017       -2.6324269582        2.6917226391
H          3.0204082208       -1.2019259242        3.6927050296

GD: psi = +-105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71482341, DF-LCCSD(T0)=-455.84123996
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0880947560
N          0.0000000000        1.3804239223        1.5414028754
C          1.2010871439       -0.7507794662        1.6598327326
H         -0.9017607258       -0.4863613099        1.4541281589
C          0.8317826515        2.2798688057        0.9425229895
H         -0.3745979493        1.5898173609        2.4514840030
N          2.2014862788       -0.9836692327        0.7729106183
O          1.2261209113       -1.1173404576        2.8325232317
C          0.8612322111        3.6631243117        1.5482119464
O          1.4991546088        1.9820934638       -0.0479918769
C          3.4581018237       -1.5512435908        1.2326369234
H          2.2098443511       -0.3856848532       -0.0409241508
H          0.5656235651        4.3803029356        0.7846604138
H          0.2061814221        3.7649887046        2.4110252955
H          1.8847120089        3.8910347576        1.8404378191
H          4.0073027317       -0.8542588387        1.8675838564
H          3.2515378906       -2.4480596579        1.8108007193
H          4.0636884900       -1.8098413630        0.3681155997

GD: psi = +-120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71387713, DF-LCCSD(T0)=-455.84044259
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0889720373
N          0.0000000000        1.3741738626        1.5529828665
C          1.2586883380       -0.7284367250        1.5562677199
H         -0.9075525302       -0.4811565876        1.4474449419
C         -0.2995202448        1.6224742811        2.8634959229
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H          0.5775497722        2.0363721936        1.0615123980
N          1.0437835257       -1.8151988572        2.3397047216
O          2.3742240043       -0.3526416172        1.2049665515
C         -0.0947547656        3.0442927432        3.3304100084
O         -0.7290635408        0.7411951816        3.6049716829
C          2.1702176965       -2.5114808821        2.9389989403
H          0.1508616523       -1.8570245742        2.8054263872
H          0.6662908740        3.0445147608        4.1092414641
H          0.2080140994        3.7156457179        2.5295212294
H         -1.0231468496        3.4013140572        3.7715068220
H          1.8140679965       -3.4347385100        3.3882329805
H          2.8963032225       -2.7430017578        2.1642098661
H          2.6617419084       -1.9013636463        3.6980713057

GD: psi = +-135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71348217, DF-LCCSD(T0)=-455.84017648
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898658789
N          0.0000000000        1.3709822833        1.5542494522
C          1.2523362879       -0.7408222036        1.5587588308
H         -0.9093311592       -0.4836837908        1.4416410719
C         -0.2340367823        1.5999589668        2.8848147837
H          0.6029723051        2.0187563230        1.0730847245
N          1.0417787925       -1.9845588079        2.0574590666
O          2.3677153637       -0.2445109576        1.4289730557
C          0.0425308145        3.0041687397        3.3673483846
O         -0.6524223960        0.7150911501        3.6258642114
C          2.1520018875       -2.7499146057        2.6000293115
H          0.1104542667       -2.1969462209        2.3750001847
H         -0.7691887689        3.3163016802        4.0198110323
H          0.9606288529        2.9893616804        3.9544050429
H          0.1536355861        3.7154152645        2.5513375666
H          1.8155914001       -3.7640486867        2.7988938288
H          2.9577205459       -2.7731350893        1.8709007568
H          2.5338454803       -2.3042864353        3.5193213046

GD: psi = +-150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71392445, DF-LCCSD(T0)=-455.84022073
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0907388664
N          0.0000000000        1.3574592279        1.5773097969
C          1.2246835076       -0.7052595713        1.6551600274
H         -0.8960827813       -0.5403456133        1.4146619145
C         -0.9374086342        2.2462790024        1.1508130538
H          0.5691647016        1.5386634908        2.3907251336
N          1.7307816373       -1.6873944748        0.8696664906
O          1.7015780678       -0.3860406723        2.7418757545
C         -0.8961983183        3.6088530124        1.8059388631
O         -1.7492622711        1.9607280231        0.2734345386
C          2.8361392544       -2.5304580992        1.2892860598
H          1.2742209613       -1.8723582926       -0.0073707149
H         -1.8563929670        3.7910791221        2.2854623421
H         -0.0995825930        3.7045571857        2.5410783244
H         -0.7645642767        4.3608347234        1.0301953481
H          3.5739739172       -2.6046083227        0.4929501431
H          3.2913127308       -2.0669184110        2.1597824753
H          2.4940390696       -3.5298100647        1.5578948426

GD: psi = +-165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71459532, DF-LCCSD(T0)=-455.84086365
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0920047344
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```
N          0.0000000000        1.3485771386        1.5949887605
C          1.2310461187       -0.7155075354        1.6344821426
H         -0.8977309269       -0.5391642540        1.4114428885
C         -1.0019279650        2.2088124148        1.2746796202
H          0.6788350811        1.5554653207        2.3128630791
N          1.5319992858       -1.8748513790        0.9996315234
O          1.8793639015       -0.2642105063        2.5755715057
C         -0.9344972054        3.5703143457        1.9297630873
O         -1.8966797793        1.8970504524        0.4912110733
C          2.6209531660       -2.7382648307        1.4204536470
H          0.9386732709       -2.1643093299        0.2402827977
H         -1.8367091884        3.7138427316        2.5219569962
H         -0.0603641601        3.6940648688        2.5659810798
H         -0.9253002593        4.3291836361        1.1497046902
H          3.2423373738       -3.0044998226        0.5675406208
H          3.2176279423       -2.1866246127        2.1411728831
H          2.2469598685       -3.6471362748        1.8913459801

GD: psi = +-180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-455.71476108, DF-LCCSD(T0)=-455.84100196
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0934608322
N          0.0000000000        1.3441924357        1.6044446764
C          1.2421826668       -0.7152447550        1.6129692192
H         -0.8989351919       -0.5356773877        1.4110011253
C         -1.0254545418        2.1923807140        1.3355403115
H          0.7737198183        1.5952846832        2.2020358354
N          1.3591522324       -2.0007667184        1.1988105705
O          2.0555166366       -0.1564983197        2.3448528498
C         -0.9193240871        3.5696345058        1.9512654733
O         -1.9759389096        1.8556734965        0.6315646591
C          2.4675493052       -2.8541380288        1.5877246841
H          0.6364186724       -2.3721694976        0.6052251315
H         -1.7834952805        3.7287043472        2.5938426064
H         -0.0079449604        3.7087341794        2.5294047949
H         -0.9585640081        4.3086654660        1.1532002602
H          2.9911300229       -3.2291218935        0.7097109688
H          3.1501339444       -2.2528906710        2.1812435729
H          2.1210148891       -3.6954402803        2.1866355388
```

6.5 ϕ profile for ADA

```
ADA: phi = +000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48355480, DF-LCCSD(T0)=-416.59080725
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0889965704
C          0.0000000000        1.4166534528        1.6473678695
H          0.8866349616       -0.5378825604        1.4294058454
H         -0.8933863234       -0.5193551750        1.4288846280
N          0.1031586096        1.3514465668        3.1080539258
C         -1.2812038406        2.1427737390        1.1836811957
H          0.8594245292        1.9740738689        1.2644452408
C         -0.7766752339        1.8442402532        4.0248456803
H          0.7530322012        0.6661371113        3.4633443918
N         -1.1211060091        3.4825186940        0.9413544300
O         -2.3032311563        1.5327038167        0.9241899487
H         -0.5409224601        1.4843625761        5.0391016449
O         -1.6946247617        2.6148033966        3.7965981246
H         -1.9892838168        3.9876710706        0.8395340764
H         -0.4136456493        3.9631891813        1.4736659258
```

```
ADA: phi = +015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48452243, DF-LCCSD(T0)=-416.59180543
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0883600564
C          0.0000000000        1.4270618521        1.6187774806
H          0.8848197027       -0.5291169094        1.4430874481
H         -0.8924176076       -0.5203069936        1.4297143814
N          0.1092368020        1.4337727005        3.0797551934
C         -1.2392633040        2.1874385006        1.1047658608
H          0.8698256810        1.9664488671        1.2330409492
C         -0.8527237391        1.7615262288        3.9860656468
H          1.0088225831        1.1896203287        3.4640780553
N         -1.1868292718        3.5470409149        1.2876870074
O         -2.1055519078        1.6349600456        0.4515177997
H         -0.4696500751        1.6993555551        5.0173333577
O         -2.0015905370        2.0816881023        3.7268681667
H         -2.0699879210        4.0136125432        1.1417112968
H         -0.6639996102        3.8823303994        2.0810096712

ADA: phi = +030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48692366, DF-LCCSD(T0)=-416.59408958
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0877459488
C          0.0000000000        1.4274803935        1.6196157188
H          0.8824560707       -0.5286643758        1.4475889211
H         -0.8939048590       -0.5191381436        1.4285845611
N          0.0755422237        1.4454588411        3.0809599194
C         -1.2167246864        2.2013785177        1.0751812096
H          0.8822597343        1.9617525466        1.2574201038
C         -0.9868510893        1.5199272463        3.9291146320
H          0.9887738073        1.4027643081        3.5046611321
N         -1.2856312742        3.5121503849        1.4732084895
O         -1.9557645390        1.7206070215        0.2350031713
H         -0.6697184469        1.5351623039        4.9839911769
O         -2.1579465230        1.5625949266        3.5871443164
H         -2.1634048246        3.9644039625        1.2665257257
H         -0.8789311216        3.7518682154        2.3623554478

ADA: phi = +045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49023083, DF-LCCSD(T0)=-416.59677537
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0891454524
C          0.0000000000        1.4444162619        1.6082955476
H          0.8841856526       -0.5263522339        1.4463607399
H         -0.8865318537       -0.5238929742        1.4449404751
N          0.0665770412        1.4505723386        3.0792622127
C         -1.1357758192        2.1985853264        0.8919927395
H          0.9024960719        1.9493989006        1.2713971306
C         -0.9025834429        1.2669384147        4.0069387997
H          0.9067394895        1.8605166141        3.4574788216
N         -2.3772535566        2.1561162376        1.4147547743
O         -0.8619321851        2.7553159115       -0.1682904450
H         -0.5331953553        1.4760894297        5.0213882564
O         -2.0473046541        0.8690941742        3.8101170777
H         -3.1108458765        2.5910802207        0.8796540755
H         -2.5751667169        1.6276804937        2.2569118120

ADA: phi = +060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49340333, DF-LCCSD(T0)=-416.59998559
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0893877661
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```
C          0.0000000000        1.4447078461        1.5994495545
H          0.8896712679       -0.5192889597        1.4433756604
H         -0.8809915427       -0.5309381688        1.4447062875
N          0.0537626430        1.4842231874        3.0666891318
C         -1.1429341722        2.2228103560        0.9242223275
H          0.9019369148        1.9473424228        1.2567783562
C         -0.8820765575        1.0659798681        3.9496663829
H          0.7968471076        2.0337985960        3.4687799903
N         -2.3882497723        2.0508078607        1.4188084406
O         -0.8877105399        2.9180335976       -0.0547565242
H         -0.5909427407        1.2795346681        4.9883289637
O         -1.9278788969        0.4822240377        3.6770794807
H         -3.1444858625        2.5017663282        0.9309524240
H         -2.5633600062        1.4066267219        2.1801218113

ADA: phi = +075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49449992, DF-LCCSD(T0)=-416.60113656
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0896150422
C          0.0000000000        1.4472978775        1.5848537181
H          0.8961208277       -0.5113909548        1.4397007559
H         -0.8736192133       -0.5398543383        1.4453178868
N          0.0722476858        1.5423496179        3.0462731344
C         -1.1613010590        2.2431911034        0.9673047536
H          0.8914597982        1.9489148135        1.2124197654
C         -0.7330453572        0.9231738112        3.9387315768
H          0.8160600335        2.0992724692        3.4350160903
N         -2.3886396500        1.9775296729        1.4716694519
O         -0.9508794187        3.0312326099        0.0514519023
H         -0.4116939259        1.0901128923        4.9770178622
O         -1.7252924580        0.2534197156        3.6628167024
H         -3.1778434391        2.4528939735        1.0668726696
H         -2.5125960845        1.2877901205        2.2016737306

ADA: phi = +090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49274515, DF-LCCSD(T0)=-416.59959413
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0896773542
C          0.0000000000        1.4505977803        1.5688420483
H          0.9003622974       -0.5058989372        1.4375544022
H         -0.8665529916       -0.5474940537        1.4470434386
N          0.1408472563        1.6065330471        3.0220942299
C         -1.2056432458        2.2364772064        1.0364026238
H          0.8607804217        1.9587590462        1.1360975133
C         -0.4270172562        0.8093697643        3.9586356780
H          0.8965965886        2.1909203983        3.3421800802
N         -2.3849405591        1.9141207325        1.6234137952
O         -1.0845173422        3.0604318389        0.1380436861
H          0.0034627646        0.9587554055        4.9597511241
O         -1.3567582010        0.0347194597        3.7534712682
H         -3.2208818677        2.3775319271        1.3094127391
H         -2.4297059804        1.2051334319        2.3422335664

ADA: phi = +105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48879756, DF-LCCSD(T0)=-416.59590101
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0897823894
C          0.0000000000        1.4550432786        1.5536639781
H          0.8995529631       -0.5057788665        1.4385348504
H         -0.8630937376       -0.5494613728        1.4504338846
N          0.1913897366        1.6544026297        2.9957488149
C         -1.2402339856        2.2086708901        1.0603967591
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H          0.8332447487        1.9652498659        1.0704057108
C         -0.0677674271        0.7493153732        3.9759243385
H          0.8344506685        2.3875481319        3.2511107589
N         -2.3765655296        1.9086562972        1.7418593093
O         -1.1914217723        2.9873248802        0.1172785620
H          0.4313547075        1.0061213307        4.9230656025
O         -0.8167744093       -0.2133709612        3.8685473350
H         -3.2422628022        2.3316952896        1.4532253113
H         -2.3736074029        1.2301006774        2.4868621448

ADA: phi = +120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48681034, DF-LCCSD(T0)=-416.59387869
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0886922229
C          0.0000000000        1.4613288367        1.5386341270
H          0.8867491375       -0.5150721930        1.4498547523
H         -0.8738918742       -0.5324881308        1.4527549135
N          0.1151073357        1.6645148332        2.9840922579
C         -1.2286639035        2.1589632840        0.9424478152
H          0.8539732364        1.9569541531        1.0725882490
C          0.1259320969        0.7400378542        3.9922718359
H          0.4480670719        2.5751703363        3.2626065442
N         -2.2596242459        2.3838637385        1.7992536646
O         -1.2543199187        2.4617151443       -0.2423876446
H          0.4318832251        1.2070161308        4.9436480521
O         -0.1847559533       -0.4358811919        3.9154321837
H         -3.1283170560        2.7155392436        1.4146411441
H         -2.2348787575        2.0256434587        2.7374040064

ADA: phi = +135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48779128, DF-LCCSD(T0)=-416.59475882
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0895766792
C          0.0000000000        1.4433003729        1.6095381659
H          0.8723817029       -0.5381955682        1.4437157556
H         -0.8893560971       -0.5260401581        1.4351861706
N         -0.0646185755        1.5561360503        3.0591796040
C         -1.2333338447        2.1836810227        1.0636085808
H          0.8916105359        1.9578320843        1.2367149098
C          0.1452479773        0.5635640760        3.9733668666
H         -0.7671119262        2.2282628064        3.3484807425
N         -1.2587662551        2.3447454468       -0.2843992941
O         -2.1113738477        2.6236146500        1.7957176902
H         -0.2889171816        0.8336335744        4.9493414827
O          0.7720565930       -0.4713243599        3.8068791374
H         -2.0753486629        2.7647084336       -0.6956549633
H         -0.5809079517        1.9111525862       -0.8838223082

ADA: phi = +150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49080910, DF-LCCSD(T0)=-416.59759761
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0896749427
C          0.0000000000        1.4433372200        1.6168553280
H          0.8731438072       -0.5355130734        1.4476622596
H         -0.8949262225       -0.5182267497        1.4351821013
N         -0.0737600672        1.5358169585        3.0655519805
C         -1.2518133486        2.1505702109        1.0820176216
H          0.8883868297        1.9656326710        1.2497906274
C          0.4376763064        0.6283983614        3.9436012721
H         -0.9108687595        2.0168303488        3.3775087951
N         -1.2330385485        2.4228497815       -0.2473517005
O         -2.1965438231        2.4455821651        1.8043121553
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H          0.0020510314        0.7517179157        4.9475298414
O          1.3076216325       -0.1972586117        3.7068188427
H         -2.0629656029        2.8062759940       -0.6673364202
H         -0.4793704782        2.1240384825       -0.8389809032

ADA: phi = +165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49367934, DF-LCCSD(T0)=-416.60034907
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898083205
C          0.0000000000        1.4413158398        1.6236439692
H          0.8803580869       -0.5268366025        1.4460687159
H         -0.8940276076       -0.5184822171        1.4372034438
N         -0.0123194812        1.5093216285        3.0719087507
C         -1.2841818307        2.1280126676        1.1529995080
H          0.8701764496        1.9764812883        1.2334145720
C          0.7934762755        0.7672162676        3.8752180145
H         -0.8874893105        1.8422183571        3.4593031291
N         -1.3062709890        2.4626693919       -0.1616613430
O         -2.2302072912        2.3280045939        1.9057979588
H          0.4735082501        0.8061995181        4.9278021878
O          1.7888638468        0.1544406627        3.5125880223
H         -2.1391266223        2.8833040104       -0.5375760100
H         -0.5104713973        2.3250746386       -0.7575308864

ADA: phi = -015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48625286, DF-LCCSD(T0)=-416.59341775
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0891208365
C          0.0000000000        1.4291242954        1.6138048751
H          0.8901098585       -0.5304421186        1.4308051111
H         -0.8944919056       -0.5136122947        1.4377099758
N          0.1167957258        1.4140818215        3.0721454685
C         -1.2878228498        2.1367596610        1.1512299984
H          0.8574450897        1.9677256417        1.1989628237
C         -0.6250465858        2.1951654741        3.9110332134
H          0.4094226766        0.5332967715        3.4696775001
N         -1.0897917760        3.2961963017        0.4518681245
O         -2.3796576676        1.6106157155        1.2878222329
H         -0.6083611175        1.8238312195        4.9470625319
O         -1.2007163057        3.2202255964        3.5842760919
H         -1.9300061783        3.8300621546        0.2851387635
H         -0.2719405140        3.8389033028        0.6756790551

ADA: phi = -030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.48980031, DF-LCCSD(T0)=-416.59695396
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0888331826
C          0.0000000000        1.4292861120        1.6141183880
H          0.8874986354       -0.5320033170        1.4331268982
H         -0.8959959597       -0.5137633080        1.4358026629
N          0.0867622277        1.4121436102        3.0699549137
C         -1.2808068027        2.1387525738        1.1413553470
H          0.8669519823        1.9653851130        1.2174058979
C         -0.4609390054        2.4025392773        3.8316447350
H          0.1092709050        0.5002550208        3.5022686226
N         -1.0803875882        3.1582135190        0.2517505468
O         -2.3838614662        1.7150729327        1.4459405535
H         -0.5616928853        2.1210051582        4.8900661494
O         -0.7626218041        3.5062601805        3.4046023622
H         -1.9064467517        3.6982344519        0.0405779235
H         -0.2279175307        3.6868036935        0.3375838698
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```
ADA: phi = -045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49269210, DF-LCCSD(T0)=-416.59987065
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0887438268
C          0.0000000000        1.4290846329        1.6148535469
H          0.8849882744       -0.5328357187        1.4365210430
H         -0.8967358973       -0.5160141247        1.4322067142
N          0.0590988431        1.4137472215        3.0678788022
C         -1.2713720839        2.1466951297        1.1326250970
H          0.8770785531        1.9637734637        1.2417561597
C         -0.2257232671        2.5469745395        3.7685817325
H         -0.1522110558        0.5404254118        3.5272069779
N         -1.0684968504        3.0930410356        0.1675134575
O         -2.3765760253        1.7939536932        1.5136297875
H         -0.3662527461        2.3695245115        4.8444360003
O         -0.2791056950        3.6586215205        3.2623828971
H         -1.8826089078        3.6414255658       -0.0669724390
H         -0.1959499095        3.5951128694        0.1885326113

ADA: phi = -060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49509041, DF-LCCSD(T0)=-416.60190450
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0876835825
C          0.0000000000        1.4245156329        1.6088155008
H          0.8841770173       -0.5279745398        1.4431440132
H         -0.8996566290       -0.5201981151        1.4144273939
N          0.0689093174        1.3963394322        3.0736883963
C         -1.2409158829        2.1947616738        1.1066270200
H          0.8893846080        1.9562414527        1.2617288936
C          0.1446433603        2.5004999866        3.8584778879
H         -0.3033329556        0.5691932605        3.5181701361
N         -1.0956897096        3.5444370282        1.0543980836
O         -2.2515166123        1.6039163832        0.7430996315
H         -0.0042741526        2.2724756823        4.9234600863
O          0.4083038923        3.6314235969        3.4627862359
H         -1.9338161040        4.0689654266        0.8558486849
H         -0.3982858632        3.9666166524        1.6543509308

ADA: phi = -075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49763442, DF-LCCSD(T0)=-416.60422869
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0876880357
C          0.0000000000        1.4245989723        1.6085241333
H          0.8826741317       -0.5288004985        1.4451127396
H         -0.8996070277       -0.5219700338        1.4121495040
N          0.0323994042        1.4116902657        3.0708622841
C         -1.2318316023        2.2030206206        1.1030139991
H          0.8974678300        1.9564060133        1.2847248172
C          0.3857499847        2.4809016927        3.8216624487
H         -0.4041760796        0.6344570197        3.5436049277
N         -1.1168071342        3.5512416410        1.2059723178
O         -2.2128963577        1.6327768692        0.6411564437
H          0.2930146818        2.2938100212        4.9006155526
O          0.7981247126        3.5466632924        3.3717642676
H         -1.9377311985        4.1004477247        1.0078391145
H         -0.3762421640        3.9435042327        1.7729532783

ADA: phi = -090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49776158, DF-LCCSD(T0)=-416.60434389
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0878645000
C          0.0000000000        1.4252346998        1.6080087957
```

```
H          0.8826604772       -0.5291213804        1.4447621942
H         -0.8990857469       -0.5230444846        1.4120538418
N          0.0052573395        1.4282005744        3.0688377445
C         -1.2298779963        2.2039458439        1.1090967522
H          0.8997629584        1.9591618275        1.2964861169
C          0.6195775200        2.3931277043        3.7905110467
H         -0.4040222081        0.6465375180        3.5566633186
N         -1.1171653250        3.5466889695        1.2802598113
O         -2.2037519409        1.6528798244        0.6132302677
H          0.6165462887        2.1935737378        4.8709744502
O          1.1249241307        3.4017364790        3.3047697787
H         -1.9258147154        4.1173415473        1.0958793020
H         -0.3461445382        3.9224939203        1.8151494269

ADA: phi = -105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49573045, DF-LCCSD(T0)=-416.60246193
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0884265563
C          0.0000000000        1.4256213646        1.6103367364
H          0.8833302255       -0.5281364933        1.4447077514
H         -0.8979436426       -0.5239237296        1.4141457788
N          0.0027848804        1.4420301999        3.0705285597
C         -1.2370577493        2.1981494598        1.1314046052
H          0.8981406577        1.9612175251        1.3005893623
C          0.8492462928        2.2331091024        3.7756036855
H         -0.4833395360        0.7057855774        3.5591101574
N         -1.0925339221        3.5470782889        1.2383539950
O         -2.2476521667        1.6482329821        0.7167652093
H          0.8537517755        2.0083012112        4.8514750072
O          1.5204029940        3.1335071288        3.2832971465
H         -1.9022379098        4.1272776736        1.0926210002
H         -0.2899042249        3.9313608861        1.7132489393

ADA: phi = -120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49496040, DF-LCCSD(T0)=-416.60174850
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0900521001
C          0.0000000000        1.4304225899        1.6362689410
H          0.8864701838       -0.5230443105        1.4445827500
H         -0.8864273039       -0.5303995422        1.4378029641
N          0.0002084093        1.4461189769        3.0843242391
C         -1.2478729425        2.1646678729        1.1488517735
H          0.9039875157        1.9522655230        1.3184756163
C          1.0109929817        2.0220874888        3.7908294940
H         -0.9052490570        1.3685180342        3.5271387459
N         -1.1303345960        2.7638927382       -0.0657218463
O         -2.2930404305        2.1426464928        1.7875033831
H          0.7810590331        2.0961541669        4.8636796824
O          2.0765152942        2.3922738979        3.3173229249
H         -1.9210275617        3.2762899463       -0.4208131375
H         -0.2298151181        2.9115703147       -0.4851685031

ADA: phi = -135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49572649, DF-LCCSD(T0)=-416.60244365
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0899846526
C          0.0000000000        1.4294673655        1.6425744368
H          0.8895072953       -0.5187281311        1.4434056068
H         -0.8837250932       -0.5333547245        1.4400206401
N          0.0249098222        1.4427242238        3.0885166821
C         -1.2556358596        2.1713113617        1.1903086889
H          0.8953468326        1.9523189876        1.2987300809
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C          1.1601401221        1.7317384350        3.7758038395
H         -0.8702702932        1.5410456722        3.5482738803
N         -1.2222966775        2.6329697066       -0.0876519139
O         -2.2395005107        2.2755207982        1.9131628234
H          0.9825835034        1.8401070323        4.8556337270
O          2.2709576393        1.8401483471        3.2729509436
H         -2.0168741468        3.1496690137       -0.4268191109
H         -0.3602123144        2.6773894859       -0.6009391268

ADA: phi = -150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49643837, DF-LCCSD(T0)=-416.60308975
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0899986288
C          0.0000000000        1.4292494973        1.6444649430
H          0.8925342753       -0.5142016661        1.4417931951
H         -0.8827356451       -0.5340318331        1.4409993507
N          0.0398716478        1.4398951765        3.0891361889
C         -1.2608174904        2.1757598734        1.2173332595
H          0.8868935001        1.9541716522        1.2796607242
C          1.2152975943        1.4251215026        3.7625245222
H         -0.8245228172        1.6621871609        3.5638489780
N         -1.2876985371        2.5579979642       -0.0860197204
O         -2.1959201788        2.3649407341        1.9865861218
H          1.0843978321        1.5286178231        4.8494442566
O          2.3134572089        1.2972346760        3.2345225209
H         -2.0868820161        3.0742410348       -0.4140572384
H         -0.4664760683        2.5131296668       -0.6619838227

ADA: phi = -165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49656477, DF-LCCSD(T0)=-416.60315853
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0900075573
C          0.0000000000        1.4316291515        1.6421154328
H          0.8916722764       -0.5147012266        1.4415835325
H         -0.8854041801       -0.5302153664        1.4404232045
N          0.0489173388        1.4477413326        3.0859163983
C         -1.2785200354        2.1569489478        1.2306026401
H          0.8735694790        1.9651486448        1.2576678289
C          1.1821961089        1.1579456391        3.7657735290
H         -0.8044406874        1.6958668346        3.5673765831
N         -1.3361561708        2.5209689337       -0.0759134904
O         -2.1975262866        2.3521361311        2.0176598653
H          1.0500940030        1.2125917017        4.8562783750
O          2.2507748963        0.8703013242        3.2388744590
H         -2.1589168060        2.9966695426       -0.4060488728
H         -0.5437560777        2.4294991887       -0.6852920439

ADA: phi = -180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49512257, DF-LCCSD(T0)=-416.60177285
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0899019966
C          0.0000000000        1.4215679088        1.6696059201
H          0.8657825903       -0.5442712147        1.4567326876
H         -0.9041282386       -0.5145949128        1.4176713968
N         -0.2432680972        1.4221773208        3.0961743446
C         -1.1068327481        2.2646069941        1.0390523217
H          0.9675541177        1.8916923947        1.4698815216
C          0.5491310893        0.7678387704        3.9780700557
H         -1.1465617966        1.7741496223        3.3855805102
N         -0.8738399943        2.6502608173       -0.2410064834
O         -2.1387069425        2.5411520448        1.6398478207
H          0.1446550298        0.7876338166        5.0011417343
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O          1.6144305569        0.2319630763        3.6972966719
H         -1.5800316578        3.1844191742       -0.7184050201
H         -0.0058117292        2.4535096522       -0.7049530400
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6.6 ψ profile for ADA

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ADA: psi = +000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49356157, DF-LCCSD(T0)=-416.60035091
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0868674824
C          0.0000000000        1.4390423788        1.5920568915
H          0.8808765090       -0.5285557822        1.4486947829
H         -0.8944574657       -0.5251193480        1.4279298993
N         -0.0464185024        1.4577386509        3.0467524876
C         -1.1304465915        2.2222004406        0.9095847918
H          0.9197808421        1.9445767553        1.2905277179
C          0.6047201358        2.4005850472        3.7863345790
H         -0.3688783981        0.6317869652        3.5268246142
N         -2.0283806175        2.8319245325        1.7280103294
O         -1.2041636144        2.2487585093       -0.3112245716
H          0.5899516971        2.1770772935        4.8642756429
O          1.1320480089        3.3987180379        3.3212794706
H         -2.6839755846        3.4618287600        1.2950892507
H         -1.8204668598        2.9455886634        2.7039954845

ADA: psi = +015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49393053, DF-LCCSD(T0)=-416.60084835
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0858799914
C          0.0000000000        1.4348569361        1.5961585621
H          0.8797538397       -0.5292773262        1.4496002475
H         -0.8968482279       -0.5228542526        1.4226979790
N         -0.0139529343        1.4254543686        3.0538446385
C         -1.1376159483        2.2320169746        0.9316190410
H          0.9199768602        1.9394711495        1.2855241131
C          0.3851418192        2.4594616085        3.8294474009
H         -0.2646530030        0.5660794225        3.5168943902
N         -1.8368333650        3.0895803383        1.7298819278
O         -1.4010496144        2.0486008938       -0.2490266298
H          0.4073341453        2.2078938943        4.8997925966
O          0.6754636021        3.5721160278        3.4023881568
H         -2.4593699939        3.7043890632        1.2268648593
H         -1.3556068747        3.4956917623        2.5188565530

ADA: psi = +030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49543844, DF-LCCSD(T0)=-416.60223994
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0859792172
C          0.0000000000        1.4304603436        1.6009106331
H          0.8792787764       -0.5296264323        1.4503546672
H         -0.8984943665       -0.5238615638        1.4157847930
N         -0.0025424439        1.4215814615        3.0600497071
C         -1.1491536495        2.2401534519        0.9670908951
H          0.9198102472        1.9391027066        1.2933899477
C          0.4482981926        2.4308492651        3.8365229735
H         -0.3171446537        0.5833628469        3.5235940035
N         -1.5990666720        3.2991271940        1.6963044533
O         -1.6242788327        1.9130151500       -0.1124358624
H          0.4531958274        2.1784363079        4.9064503568
O          0.8065597107        3.5264081449        3.4125784449
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H         -2.2355596228        3.9112949687        1.2090336157
H         -0.9695783204        3.7218793230        2.3660532920

ADA: psi = +045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49682318, DF-LCCSD(T0)=-416.60348082
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0864178199
C          0.0000000000        1.4271876167        1.6049426163
H          0.8801436222       -0.5292873615        1.4492384692
H         -0.8990869264       -0.5247229965        1.4112252778
N          0.0068669793        1.4197417705        3.0651366922
C         -1.1757003860        2.2323597549        1.0139791970
H          0.9141343862        1.9443243451        1.2965738982
C          0.5022203107        2.4168809057        3.8294868161
H         -0.3569335379        0.6051299629        3.5349793046
N         -1.3918497769        3.4364930218        1.6043470685
O         -1.8569544697        1.7926622416        0.0964590599
H          0.4907304687        2.1805957045        4.9026863949
O          0.9214796335        3.4858667170        3.3922742433
H         -2.0734546733        4.0373723580        1.1697557157
H         -0.6740301363        3.8427457884        2.1903658973

ADA: psi = +060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49769723, DF-LCCSD(T0)=-416.60424067
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0870865072
C          0.0000000000        1.4254078228        1.6073306861
H          0.8814690188       -0.5291046405        1.4471165285
H         -0.8994000664       -0.5240255576        1.4101070995
N          0.0114453817        1.4188479852        3.0683803968
C         -1.2060787168        2.2174826943        1.0627935725
H          0.9066813859        1.9513691611        1.2964362983
C          0.5209383677        2.4202292862        3.8187224958
H         -0.3775615975        0.6197904016        3.5448178277
N         -1.2289265420        3.5165379023        1.4478946084
O         -2.0603128552        1.6978897502        0.3552512464
H          0.4962678133        2.2049879045        4.8959754162
O          0.9706920503        3.4698745794        3.3650920292
H         -1.9832316507        4.0968602507        1.1212667978
H         -0.4753653403        3.9053526111        1.9985233742

ADA: psi = +075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49801632, DF-LCCSD(T0)=-416.60458323
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0877722026
C          0.0000000000        1.4249578930        1.6080026742
H          0.8826112368       -0.5290517985        1.4447892403
H         -0.8993290847       -0.5224384146        1.4120776137
N          0.0088555978        1.4205881203        3.0697579146
C         -1.2274147682        2.2054080657        1.1020551518
H          0.9016284170        1.9561820735        1.2963826268
C          0.4977936108        2.4434800930        3.8063345726
H         -0.4107604733        0.6402739768        3.5512007940
N         -1.1043267074        3.5520382936        1.2269146552
O         -2.2095403324        1.6456862730        0.6314474761
H          0.4507414451        2.2561806173        4.8879214955
O          0.9561659270        3.4815079182        3.3355646600
H         -1.9215952612        4.1125056703        1.0471245337
H         -0.3504688080        3.9306146834        1.7854577317

ADA: psi = +090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49740277, DF-LCCSD(T0)=-416.60410207
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```
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0885472191
C          0.0000000000        1.4255843294        1.6095268629
H          0.8839145695       -0.5287790425        1.4427978707
H         -0.8988770639       -0.5203544474        1.4171659682
N          0.0453857146        1.4243676589        3.0689088479
C         -1.2619899755        2.1794806557        1.1571315989
H          0.8845946491        1.9668778776        1.2722548664
C          0.4962825507        2.4942306153        3.7668635231
H         -0.4161861800        0.6797891049        3.5685486134
N         -1.0675465930        3.5146069157        0.9768327694
O         -2.3273377349        1.6077835956        0.9653639645
H          0.4456298996        2.3526614894        4.8553981274
O          0.9388123279        3.5175548641        3.2529705129
H         -1.8925969297        4.0777625190        0.8390942195
H         -0.2693063681        3.9408655027        1.4278973389

ADA: psi = +105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49614096, DF-LCCSD(T0)=-416.60301385
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0889461943
C          0.0000000000        1.4267510888        1.6124489452
H          0.8839220924       -0.5293163076        1.4421194286
H         -0.8983052763       -0.5186726710        1.4223540641
N          0.0454766409        1.4242953485        3.0686639882
C         -1.2701192580        2.1630504510        1.1595385914
H          0.8830742559        1.9669514894        1.2719391898
C          0.4440647277        2.5293452991        3.7483764422
H         -0.4520892303        0.7030958599        3.5680675377
N         -1.0490851853        3.4158837878        0.6695039128
O         -2.3710622178        1.6309029213        1.2081982288
H          0.3682783264        2.4174759809        4.8391003074
O          0.8705346832        3.5473964917        3.2140973951
H         -1.8696613780        3.9803676090        0.5078869052
H         -0.2174925122        3.8947927451        0.9828593154

ADA: psi = +120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49508608, DF-LCCSD(T0)=-416.60208653
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0891602905
C          0.0000000000        1.4286595868        1.6146205200
H          0.8834261723       -0.5303015627        1.4417768586
H         -0.8973258713       -0.5184332259        1.4264434057
N          0.0330841621        1.4245075350        3.0680853796
C         -1.2661668947        2.1514564235        1.1358021834
H          0.8882860004        1.9631988573        1.2789089143
C          0.3617333797        2.5587256333        3.7413938696
H         -0.4953199432        0.7173939427        3.5559485742
N         -1.0430389683        3.2500514575        0.3595445968
O         -2.3792148139        1.7133465047        1.3927616871
H          0.2542895840        2.4617839169        4.8309778051
O          0.7679682527        3.5809564928        3.2025366789
H         -1.8538839812        3.8077431984        0.1375681523
H         -0.1733899195        3.7432678197        0.4847174456

ADA: psi = +135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49531560, DF-LCCSD(T0)=-416.60197143
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0906293417
C          0.0000000000        1.4320112969        1.6314709600
H          0.8915700419       -0.5158442752        1.4426142629
H         -0.8878943702       -0.5238619183        1.4426255413
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N          0.0208648981        1.4697437888        3.0810817399
C         -1.2683683856        2.1544775513        1.1919960622
H          0.8918350797        1.9548076382        1.2820529270
C          1.1714641526        1.3088447730        3.7799189696
H         -0.8696471169        1.4573413045        3.5572167524
N         -1.1205878339        3.0340395418        0.1689803888
O         -2.3440320750        1.9286610412        1.7340906743
H          1.0093123636        1.3047404480        4.8679623816
O          2.2806062361        1.2001493627        3.2723273872
H         -1.9325819377        3.5269866030       -0.1642792644
H         -0.2169178463        3.2607534981       -0.2041426199

ADA: psi = +150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49625204, DF-LCCSD(T0)=-416.60285365
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0903835979
C          0.0000000000        1.4324094361        1.6363283114
H          0.8921518700       -0.5142255472        1.4427925333
H         -0.8853678703       -0.5281522028        1.4431187558
N          0.0264481609        1.4600207636        3.0824188041
C         -1.2670310702        2.1572578745        1.1969768328
H          0.8882060602        1.9560806225        1.2757735435
C          1.1774992452        1.2989775084        3.7764977596
H         -0.8549820605        1.5947095175        3.5570666730
N         -1.1877603307        2.7858577617       -0.0031852319
O         -2.2865790722        2.1369217221        1.8768275760
H          1.0283754484        1.3483505946        4.8650300579
O          2.2757777069        1.1228213717        3.2625582996
H         -2.0065738632        3.2483967103       -0.3613678866
H         -0.3236160660        2.8493949200       -0.5097675623

ADA: psi = +165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49662012, DF-LCCSD(T0)=-416.60322475
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0900033264
C          0.0000000000        1.4304831896        1.6438222496
H          0.8923028979       -0.5140837602        1.4415151348
H         -0.8843076035       -0.5317436617        1.4407321594
N          0.0482991954        1.4422586322        3.0876046996
C         -1.2732616694        2.1637131155        1.2305687396
H          0.8773461952        1.9615646302        1.2645573540
C          1.2032800819        1.2350992155        3.7616543705
H         -0.8040116166        1.6919015457        3.5701072522
N         -1.3267939692        2.5278949779       -0.0762839414
O         -2.1931321046        2.3624817402        2.0157382906
H          1.0790494771        1.3070320803        4.8520071849
O          2.2799604960        0.9910858635        3.2294080852
H         -2.1439277810        3.0139595455       -0.4054375136
H         -0.5297064318        2.4428296046       -0.6805295594

ADA: psi = -015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49264232, DF-LCCSD(T0)=-416.59952007
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0881557858
C          0.0000000000        1.4490880720        1.5874040037
H          0.8890102619       -0.5171114229        1.4468884791
H         -0.8829780188       -0.5247495951        1.4477378971
N          0.0574918207        1.5199044494        3.0480870517
C         -1.1456151928        2.2152332460        0.9064294728
H          0.9016901302        1.9446155503        1.2289161882
C         -0.8203974953        0.9765002756        3.9218608359
H          0.8798292677        1.9352564106        3.4551901649
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N         -2.1826371773        2.6318020641        1.6845185759
O         -1.0489770330        2.4633260399       -0.2885862911
H         -0.4795411032        1.0625755225        4.9642833039
O         -1.8939211599        0.4627326670        3.6210917150
H         -2.9603720570        3.0149176790        1.1677893632
H         -2.4088347852        2.0777044916        2.5001442345

ADA: psi = -030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49384426, DF-LCCSD(T0)=-416.60056955
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0887991189
C          0.0000000000        1.4498457615        1.5855645172
H          0.8916387400       -0.5151373402        1.4440597069
H         -0.8794073386       -0.5298565645        1.4483446875
N          0.0735139148        1.5300077869        3.0461061903
C         -1.1615017415        2.2090184559        0.9253551484
H          0.8933230158        1.9489773074        1.2136014761
C         -0.7578597107        0.9492649153        3.9403992783
H          0.8558726372        2.0292666706        3.4375343617
N         -2.3052890783        2.3389062858        1.6462014624
O         -1.0072796287        2.6637215114       -0.2018166930
H         -0.4135849686        1.0825814471        4.9764296709
O         -1.7938314940        0.3491499076        3.6665773324
H         -3.0953476446        2.7137187997        1.1444506088
H         -2.4789194166        1.6950100233        2.4081121524

ADA: psi = -045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49445047, DF-LCCSD(T0)=-416.60109552
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0894255393
C          0.0000000000        1.4487350047        1.5846890605
H          0.8942904555       -0.5132059892        1.4412719853
H         -0.8759331657       -0.5357985872        1.4468466510
N          0.0881329773        1.5390999757        3.0446731667
C         -1.1725964981        2.2204966435        0.9586628141
H          0.8858591986        1.9526636734        1.2020259619
C         -0.7148571301        0.9341405159        3.9488866732
H          0.8369590902        2.0950704085        3.4252250734
N         -2.3738308777        2.0827202368        1.5695140122
O         -0.9894703381        2.8910383820       -0.0513261362
H         -0.3799132798        1.1037729766        4.9825485447
O         -1.7161177708        0.2722939307        3.6873286694
H         -3.1714763591        2.4957480560        1.1145332632
H         -2.5011976623        1.3936332196        2.2999513162

ADA: psi = -060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49445664, DF-LCCSD(T0)=-416.60111441
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0897468230
C          0.0000000000        1.4458102026        1.5873960444
H          0.8962437970       -0.5114395153        1.4396268699
H         -0.8735720820       -0.5410384390        1.4436215516
N          0.0589224165        1.5350477908        3.0504249324
C         -1.1529137710        2.2581028784        0.9735427996
H          0.8961575565        1.9472400512        1.2262844240
C         -0.7788127856        0.9423176656        3.9313633361
H          0.7961787488        2.0939562295        3.4489193762
N         -2.3968177114        1.9049156165        1.3743626505
O         -0.9219824796        3.1285123904        0.1407018451
H         -0.4790248924        1.1185694977        4.9746363399
O         -1.7716425088        0.2794064138        3.6416121672
H         -3.1734559219        2.4349614616        1.0151925757
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H         -2.5275951591        1.2268526061        2.1143612880

ADA: psi = -075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49389537, DF-LCCSD(T0)=-416.60072636
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0897162935
C          0.0000000000        1.4423079553        1.5906995922
H          0.8984262099       -0.5081767747        1.4390836673
H         -0.8691565194       -0.5487376867        1.4410865009
N          0.0445489275        1.5308285542        3.0546804813
C         -1.1415236464        2.2964040453        1.0122875215
H          0.9021335430        1.9421231801        1.2415663277
C         -0.8375607012        0.9589642468        3.9067898470
H          0.7573249744        2.1105802768        3.4674332841
N         -2.3892522854        1.7822593816        1.1649563067
O         -0.8991824914        3.3367153220        0.4104856037
H         -0.5842061041        1.1471337827        4.9602215177
O         -1.8180645631        0.2954817268        3.5801639073
H         -3.1573589274        2.3747728152        0.8920654950
H         -2.5416555508        1.0719954509        1.8702072664

ADA: psi = -090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49254852, DF-LCCSD(T0)=-416.59963308
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0894537847
C          0.0000000000        1.4387270453        1.5963084185
H          0.8999623438       -0.5052401887        1.4390006770
H         -0.8642837754       -0.5560696208        1.4412565330
N          0.0266045394        1.5198683554        3.0598533245
C         -1.1235266086        2.3343413920        1.0425313510
H          0.9110017129        1.9337941858        1.2623386460
C         -0.9299499288        1.0001680408        3.8666481293
H          0.7118077636        2.1192642115        3.4906849445
N         -2.3391045683        1.7370895330        0.8959890599
O         -0.8862943832        3.4886406716        0.7074960391
H         -0.7358055969        1.1968823621        4.9311784458
O         -1.9079597657        0.3647649274        3.4850582088
H         -3.1004276238        2.3592790951        0.6693766470
H         -2.5468515968        0.9598060840        1.5089247336

ADA: psi = -105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49102916, DF-LCCSD(T0)=-416.59833232
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0891454087
C          0.0000000000        1.4342869550        1.6069667164
H          0.8994506924       -0.5059273111        1.4380952236
H         -0.8611892387       -0.5593217399        1.4455244791
N          0.0147294268        1.4934806457        3.0699396566
C         -1.1124441093        2.3584911987        1.0757410154
H          0.9176107480        1.9268580924        1.2859818108
C         -1.0165250265        1.0418369218        3.8275959241
H          0.6750581442        2.1096335175        3.5155642259
N         -2.2411357624        1.7491278369        0.6136354679
O         -0.9297805269        3.5683220543        1.0325339976
H         -0.8740955318        1.2405554765        4.8999295066
O         -2.0004249669        0.4563181248        3.3902574325
H         -3.0077714899        2.3750258901        0.4157197047
H         -2.4874562247        0.8661994628        1.0351359997

ADA: psi = -120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49036076, DF-LCCSD(T0)=-416.59772287
H          0.0000000000        0.0000000000        0.0000000000
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C          0.0000000000        0.0000000000        1.0893749627
C          0.0000000000        1.4307119663        1.6185358358
H          0.8980513065       -0.5101870206        1.4345392313
H         -0.8623826798       -0.5556735230        1.4523102657
N          0.0229016820        1.4654003130        3.0787180198
C         -1.1256534089        2.3563824061        1.1137691393
H          0.9142927054        1.9289515531        1.2939134407
C         -1.0593284135        1.0891921388        3.8083117448
H          0.6969869172        2.0591878632        3.5336044262
N         -2.1104594582        1.7803406351        0.3674465798
O         -1.0642594735        3.5579433876        1.3341035341
H         -0.9342774007        1.2736816065        4.8852981890
O         -2.0658854709        0.5774520551        3.3349772441
H         -2.9014044540        2.3778763017        0.1793004275
H         -2.3195365988        0.8100544853        0.5359550740

ADA: psi = -135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49196604, DF-LCCSD(T0)=-416.59893107
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0915651535
C          0.0000000000        1.4247189604        1.6390208967
H          0.9074462839       -0.5022733878        1.4174577274
H         -0.8619945072       -0.5567972628        1.4590329555
N          0.1374321281        1.4256040491        3.0893598474
C         -1.2605031497        2.2453266140        1.3404801456
H          0.8431492424        1.9725766382        1.2021227459
C          1.3348522444        1.1368997247        3.6700576769
H         -0.4706546204        2.0622870085        3.5872586622
N         -2.1245262091        1.7329842712        0.4281242185
O         -1.4859569829        3.2856488304        1.9488766715
H          1.3340845108        1.3285398231        4.7535788959
O          2.3052326662        0.6859931765        3.0775602851
H         -2.9071833231        2.3051921332        0.1566411339
H         -1.9044465288        0.9170250483       -0.1122313818

ADA: psi = -150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49372560, DF-LCCSD(T0)=-416.60059226
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0913215929
C          0.0000000000        1.4224994676        1.6503475273
H          0.9101000184       -0.5004480159        1.4134832668
H         -0.8632346969       -0.5573164637        1.4535385407
N          0.1959591090        1.4161760178        3.0891773230
C         -1.2903849319        2.2104954046        1.3991525010
H          0.8175934851        1.9845184869        1.1826145843
C          1.4245894268        1.1750730782        3.6188904879
H         -0.4448554576        1.9928636233        3.6191282271
N         -2.0115209167        1.8548434898        0.3057937132
O         -1.6592091509        3.0882118044        2.1718432610
H          1.4574409402        1.3451006195        4.7052932048
O          2.3922181263        0.7838851281        2.9794916479
H         -2.8006702391        2.4301052924        0.0616490269
H         -1.6746585501        1.1813946342       -0.3568024179

ADA: psi = -165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49519826, DF-LCCSD(T0)=-416.60196501
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0905568836
C          0.0000000000        1.4215937907        1.6582342210
H          0.9056719198       -0.5045428353        1.4195655329
H         -0.8699628713       -0.5515652156        1.4449987319
N          0.1804346756        1.4067352815        3.0951921346
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C          -1.2985216172        2.1865987970        1.3879419974
H           0.8239762460        1.9832625638        1.2031226386
C           1.4080045442        1.2047914487        3.6378037329
H          -0.5231613072        1.8986880688        3.6310970472
N          -1.8171777420        2.0476948623        0.1408909612
O          -1.8477747825        2.8556921903        2.2561778522
H           1.4189897129        1.3461424098        4.7284850623
O           2.4012610951        0.8762904891        3.0010662809
H          -2.6154768083        2.6116676207       -0.0986377289
H          -1.3281824015        1.5604184825       -0.5869131221

ADA: psi = -180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-416.49614619, DF-LCCSD(T0)=-416.60281773
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0900363160
C           0.0000000000        1.4357720898        1.6288062727
H           0.9055067973       -0.4994272933        1.4279601080
H          -0.8727517806       -0.5440093702        1.4491486976
N           0.2077346218        1.4762612729        3.0577974254
C          -1.3272236482        2.1422437271        1.3511180069
H           0.8082906506        1.9923613024        1.1429535111
C           1.4388934495        1.3063865505        3.5958353929
H          -0.5516236478        1.8489757887        3.6121576368
N          -1.6885496778        2.2001586083        0.0426870938
O          -2.0345699976        2.5805480681        2.2510454793
H           1.4497161098        1.4448048268        4.6868146384
O           2.4411344842        1.0180784914        2.9523650348
H          -2.5202117350        2.7152973416       -0.1932276316
H          -1.0537801988        1.9413015894       -0.6906229584
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6.7 ϕ profile for AD

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AD: phi = +000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.92862667, DF-LCCSD(T0)=-495.07503503
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0891552154
C           0.0000000000        1.4091604820        1.6677997854
H           0.8848058364       -0.5446206907        1.4253076933
H          -0.8950103382       -0.5193056170        1.4254841206
N           0.0929379260        1.3079337964        3.1294078363
C          -1.2887359073        2.1277212028        1.2216386918
H           0.8594269192        1.9758454250        1.2987065490
C          -0.8189853557        1.7739644223        4.0412862161
H           0.6790824742        0.5541203561        3.4537505365
N          -1.1439998238        3.4598930068        0.9716239668
O          -2.3251465561        1.5133652059        1.0124764496
C          -0.6798761854        1.1803624826        5.4284793512
O          -1.6711628768        2.6135607852        3.7777153224
C          -2.3497928037        4.2609168939        0.8191079220
H          -0.3652341092        3.9025024935        1.4331841266
H          -0.8788442249        1.9578611935        6.1611136491
H           0.3014479413        0.7453551806        5.6109273304
H          -1.4359475778        0.4035457960        5.5444504769
H          -2.9441593161        4.2447436355        1.7343291212
H          -2.9473079879        3.8532248739        0.0084776663
H          -2.0652093768        5.2817278384        0.5769144921

AD: phi = +015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.92919205, DF-LCCSD(T0)=-495.07566276
H           0.0000000000        0.0000000000        0.0000000000
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```
C          0.0000000000        0.0000000000        1.0885507046
C          0.0000000000        1.4268830420        1.6199545001
H          0.8844108887       -0.5307152482        1.4428876911
H         -0.8934982597       -0.5191903549        1.4290491812
N          0.1012421153        1.4302059951        3.0826563310
C         -1.2371310700        2.1874989894        1.1038510389
H          0.8756176019        1.9619313999        1.2406290156
C         -0.8733495222        1.7572139914        3.9844598181
H          0.9922498904        1.1531081204        3.4612735861
N         -1.1881668258        3.5396483975        1.2936086308
O         -2.1174681232        1.6306109449        0.4660548695
C         -0.4552443351        1.6514492357        5.4378009776
O         -2.0053085091        2.1020117245        3.6645294911
C         -2.4149231213        4.3014310929        1.1073460401
H         -0.5886209618        3.8423407063        2.0454662989
H         -0.6670363203        2.6006178113        5.9262346514
H          0.5950555138        1.4004615145        5.5746071339
H         -1.0704998176        0.8898447750        5.9141832854
H         -3.1781207357        3.9959520455        1.8253949828
H         -2.7907902684        4.1282058615        0.1029593635
H         -2.1933663885        5.3588806451        1.2288749443

AD: phi = +030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93151774, DF-LCCSD(T0)=-495.07789167
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0878348504
C          0.0000000000        1.4274139906        1.6213609445
H          0.8815409888       -0.5301493589        1.4483912882
H         -0.8954035186       -0.5172227821        1.4280033194
N          0.0636621607        1.4408932069        3.0841633235
C         -1.2149200481        2.2001429726        1.0704005195
H          0.8889933468        1.9569267062        1.2687659630
C         -1.0164142909        1.5102858253        3.9200886873
H          0.9767114600        1.4157249160        3.5067116696
N         -1.3082752179        3.4952681624        1.4933473344
O         -1.9491365913        1.7199839418        0.2202315385
C         -0.6878643156        1.5313805229        5.3989693234
O         -2.1713970997        1.5428001339        3.5104525646
C         -2.5422409191        4.2212208284        1.2307024518
H         -0.8390058023        3.7025202483        2.3603239056
H         -1.1533411492        2.4093354890        5.8432444459
H          0.3802741598        1.5433009093        5.6081450959
H         -1.1340452448        0.6520698105        5.8604985654
H         -3.3844298856        3.7728265091        1.7609684054
H         -2.7495446990        4.1947796478        0.1646332877
H         -2.4161476763        5.2542241679        1.5455510474

AD: phi = +045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93523598, DF-LCCSD(T0)=-495.08183689
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0903344370
C          0.0000000000        1.4250630910        1.6373498677
H          0.8971761795       -0.5157665192        1.4288490373
H         -0.8647313361       -0.5507996433        1.4590308113
N          0.0805070877        1.4227268824        3.0963837239
C         -1.1781472939        2.3191733217        1.2005937387
H          0.8918065559        1.9445182751        1.2814267461
C         -1.0692549096        1.2712056156        3.8285597757
H          0.7865351421        2.0115628145        3.5082638369
N         -2.0346411273        1.8119204386        0.2785253681
O         -1.2633463651        3.4660623022        1.6288315334
C         -0.9735680305        1.6661220807        5.2829031953
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O         -2.1002246246        0.8388777845        3.3225001768
C         -3.2360104915        2.5640258676       -0.0491785333
H         -2.0781065754        0.8099388184        0.2034016358
H         -1.6234126434        1.0217583364        5.8683484579
H         -1.3298759575        2.6926102062        5.3777572491
H          0.0449678299        1.6114283988        5.6633390509
H         -3.7574925615        2.0558514954       -0.8562290456
H         -2.9556899285        3.5627012632       -0.3732563307
H         -3.8942457622        2.6550935124        0.8160288042

AD: phi = +060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93807844, DF-LCCSD(T0)=-495.08374675
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0896068973
C          0.0000000000        1.4445153588        1.5999746031
H          0.8891359528       -0.5211085261        1.4432526540
H         -0.8819667006       -0.5291703522        1.4449328171
N          0.0569058532        1.4851165954        3.0683398076
C         -1.1336365422        2.2312498853        0.9189231496
H          0.9053600240        1.9437789528        1.2599556811
C         -0.8893923369        1.0738881407        3.9517846325
H          0.8005103722        2.0409713178        3.4572997098
N         -2.3854322182        2.0539817594        1.3814669315
O         -0.8660323537        2.9442923587       -0.0506060652
C         -0.5770615827        1.3387919755        5.4083781466
O         -1.9266800109        0.4918537374        3.6225384921
C         -3.5028586458        2.7087061200        0.7262419769
H         -2.5276266158        1.4048373835        2.1478443053
H         -0.5883151423        0.3879146116        5.9378979580
H         -1.3715279718        1.9578576313        5.8217717799
H          0.3817809642        1.8281610558        5.5663750259
H         -4.4080406411        2.4869459988        1.2852864152
H         -3.6145230927        2.3580893976       -0.2998147434
H         -3.3483638224        3.7862548101        0.6976765232

AD: phi = +075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93921659, DF-LCCSD(T0)=-495.08496003
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898220000
C          0.0000000000        1.4469317069        1.5849393209
H          0.8959119005       -0.5129531183        1.4392220689
H         -0.8742475686       -0.5387151216        1.4452027746
N          0.0756391491        1.5460299799        3.0476086186
C         -1.1521713336        2.2540171122        0.9657291204
H          0.8949617285        1.9450873164        1.2149955837
C         -0.7410594932        0.9351193252        3.9429955786
H          0.8292736479        2.0964988073        3.4229885203
N         -2.3873614639        1.9741377400        1.4286510784
O         -0.9301211885        3.0731947058        0.0730770325
C         -0.3686684776        1.1135091897        5.3980544348
O         -1.7338379357        0.2793182701        3.6142035757
C         -3.5463108970        2.6651699266        0.8950046704
H         -2.4775866772        1.2821843191        2.1643265045
H         -1.2134210065        1.5624162654        5.9171790915
H          0.5168096855        1.7279798773        5.5474943300
H         -0.1996870622        0.1284349778        5.8297616381
H         -4.4334497966        2.2930810598        1.4004482556
H         -3.6392665290        2.4902208460       -0.1762941436
H         -3.4627757453        3.7398988874        1.0540297928

AD: phi = +090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93728302, DF-LCCSD(T0)=-495.08323308
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H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0899239191
C          0.0000000000        1.4506396727        1.5687366351
H          0.9015387856       -0.5059201935        1.4362941971
H         -0.8661837904       -0.5480235540        1.4470981247
N          0.1456828977        1.6110372466        3.0223805349
C         -1.1940405710        2.2494178635        1.0261111418
H          0.8653085795        1.9534563918        1.1377552208
C         -0.4378753393        0.8188878038        3.9622752462
H          0.9230411540        2.1730452682        3.3271134845
N         -2.3814808045        1.9211992610        1.5864213690
O         -1.0451826467        3.0858042476        0.1369440048
C          0.1411069828        0.9154584709        5.3559571073
O         -1.3964029359        0.0859439429        3.7083064349
C         -3.6220613658        2.5685292119        1.2056306419
H         -2.3730328309        1.2204144263        2.3188017914
H         -0.6755882767        0.9436478521        6.0728026536
H          0.7812557952        1.7850976090        5.4923448784
H          0.7253145837        0.0151919284        5.5465997965
H         -4.3999670204        1.8230356970        1.0500046638
H         -3.4487794490        3.1090780057        0.2788970007
H         -3.9539056809        3.2744287748        1.9678944252

AD: phi = +105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93322623, DF-LCCSD(T0)=-495.07950645
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0901036356
C          0.0000000000        1.4549362000        1.5524824484
H          0.9016977573       -0.5050864601        1.4363934981
H         -0.8620237715       -0.5511515138        1.4499683636
N          0.1963116867        1.6674136347        2.9952729870
C         -1.2302229263        2.2260519163        1.0589256117
H          0.8369702911        1.9599240621        1.0694720598
C         -0.0861275236        0.7555201718        3.9722453317
H          0.9016590044        2.3485946979        3.2258299732
N         -2.3735563612        1.8910813742        1.7063582046
O         -1.1571003633        3.0427216071        0.1441658569
C          0.6558486276        0.9488577484        5.2767185404
O         -0.9170178743       -0.1383225693        3.8176338159
C         -3.6507927731        2.5086321778        1.4068601389
H         -2.3039939636        1.2149844111        2.4548847322
H          0.0040678266        0.6639925057        6.0978775454
H          0.9998991428        1.9726257175        5.4153031997
H          1.5230077611        0.2876881383        5.2828235875
H         -4.4165156833        1.7465352991        1.2713819763
H         -3.5379089638        3.0731646245        0.4851367879
H         -3.9607890422        3.1880289109        2.2014839091

AD: phi = +120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93070190, DF-LCCSD(T0)=-495.07692780
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0888770009
C          0.0000000000        1.4621697418        1.5345226195
H          0.8878971867       -0.5148669424        1.4494358169
H         -0.8730054510       -0.5326019188        1.4536342664
N          0.1331106104        1.6863199907        2.9781659124
C         -1.2283749020        2.1610081508        0.9367673287
H          0.8524043465        1.9525765592        1.0586487250
C          0.1442242454        0.7548219701        3.9917163383
H          0.5625476717        2.5660954128        3.2178290166
N         -2.2310499422        2.4328449313        1.8062951866
O         -1.2700114482        2.4112515784       -0.2647299161
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C          0.7215678853        1.2715995619        5.2965103030
O         -0.2812713974       -0.3864949179        3.8814757549
C         -3.5025971994        2.9780610885        1.3708940414
H         -2.1023461706        2.1430652060        2.7618503210
H          0.2069368175        0.7859316517        6.1208426295
H          0.6438298787        2.3532400630        5.3986009424
H          1.7752688077        0.9943264333        5.3414425642
H         -4.2623243944        2.2002437253        1.2871395879
H         -3.3541863631        3.4274879962        0.3926722618
H         -3.8433623428        3.7375125861        2.0718670313

AD: phi = +135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93156270, DF-LCCSD(T0)=-495.07775771
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0900435373
C          0.0000000000        1.4457107192        1.6043717506
H          0.8699880269       -0.5397951461        1.4472003787
H         -0.8922469320       -0.5227759939        1.4341252624
N         -0.0970848107        1.5773116862        3.0520512598
C         -1.2234774431        2.1809705101        1.0261940029
H          0.9025161580        1.9511145276        1.2453109684
C          0.0963573060        0.5797129961        3.9760160050
H         -0.8360535147        2.2257074318        3.3000208298
N         -1.2101461951        2.3692950350       -0.3129789335
O         -2.1459872162        2.5834566609        1.7333317982
C         -0.5831270716        0.8381944340        5.3068502766
O          0.7776091653       -0.4208157325        3.7831203283
C         -2.3331926639        2.9979228856       -0.9882430791
H         -0.4555473798        1.9862245745       -0.8544827302
H          0.0290845178        0.4164333386        6.0990507824
H         -1.5464681410        0.3269125785        5.3076388189
H         -0.7539113749        1.8972194459        5.4918379838
H         -2.0845743735        3.1151251303       -2.0394845288
H         -2.5311146333        3.9750257828       -0.5523366105
H         -3.2341944586        2.3927313738       -0.8941192986

AD: phi = +150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93484902, DF-LCCSD(T0)=-495.08087929
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0902013830
C          0.0000000000        1.4457793592        1.6123584823
H          0.8713048892       -0.5371773693        1.4501212699
H         -0.8982869508       -0.5138453921        1.4347482250
N         -0.0890437474        1.5516846967        3.0607481698
C         -1.2542124210        2.1375140744        1.0618410918
H          0.8917714646        1.9647571653        1.2493040524
C          0.4325173014        0.6394725650        3.9407056632
H         -0.9623346136        1.9821896413        3.3445598780
N         -1.2051151374        2.4705612198       -0.2476839246
O         -2.2436612839        2.3571799001        1.7591067479
C         -0.1958197519        0.6705267028        5.3190752862
O          1.3523028339       -0.1232675126        3.6624243907
C         -2.3615533738        3.0422414757       -0.9169725861
H         -0.3811860678        2.2463653267       -0.7777393862
H          0.5714266074        0.4575679786        6.0583778423
H         -0.9493451730       -0.1160442874        5.3726062063
H         -0.6724490649        1.6236344026        5.5408443972
H         -2.0850724821        3.2880241256       -1.9385859518
H         -2.6825597046        3.9455806958       -0.4021576547
H         -3.1938620453        2.3394125655       -0.9257215968

AD: phi = +165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
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DF-LMP2=-494.93772660, DF-LCCSD(T0)=-495.08359017
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0903625644
C          0.0000000000        1.4420760693        1.6229287795
H          0.8793665762       -0.5284766334        1.4466436563
H         -0.8963794285       -0.5154938540        1.4370465115
N         -0.0261001135        1.5141747914        3.0720306674
C         -1.2862186870        2.1185111754        1.1402483899
H          0.8744036314        1.9751073838        1.2401446819
C          0.7893026999        0.7692780908        3.8745060623
H         -0.9260003719        1.8008849839        3.4371147111
N         -1.2595571064        2.5307383565       -0.1501105352
O         -2.2670194445        2.2385821008        1.8721289459
C          0.3703947994        0.7041444903        5.3280768822
O          1.8034621275        0.2113555325        3.4630316668
C         -2.4178841506        3.0983778220       -0.8167893673
H         -0.4092716786        2.3960617009       -0.6705895490
H          1.2508102803        0.8420224165        5.9509393415
H         -0.0281922074       -0.2908394715        5.5259440421
H         -0.3839855284        1.4449070469        5.5858589392
H         -2.1584146483        4.0451749618       -1.2869320364
H         -3.1795050946        3.2696866182       -0.0615986709
H         -2.8120774635        2.4178425605       -1.5711936637

AD: phi = -015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93188350, DF-LCCSD(T0)=-495.07828199
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0892995629
C          0.0000000000        1.4286733682        1.6147766936
H          0.8893689372       -0.5322218907        1.4308730307
H         -0.8954107644       -0.5132527193        1.4370608053
N          0.1263605378        1.4104112435        3.0742707780
C         -1.2892414250        2.1368890962        1.1684540991
H          0.8549035686        1.9684765549        1.1945130156
C         -0.6251079199        2.2037002540        3.9080225870
H          0.3616795877        0.5058347365        3.4555610488
N         -1.1066816205        3.2974485064        0.4813294794
O         -2.3856537009        1.6174163835        1.3369252479
C         -0.7567489425        1.6932856345        5.3258321904
O         -1.1279374299        3.2570375462        3.5358113318
C         -2.2701966698        4.1267624668        0.2062908969
H         -0.2390792961        3.7760829143        0.6622547428
H         -0.8616157610        2.5405793716        5.9972978046
H          0.0929462022        1.0830370520        5.6290325144
H         -1.6617850254        1.0877054769        5.3889475511
H         -2.7189914134        4.4908094259        1.1320873178
H         -3.0094422244        3.5358077919       -0.3274903563
H         -1.9649746956        4.9661761546       -0.4134250000

AD: phi = -030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93553603, DF-LCCSD(T0)=-495.08194425
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0890127352
C          0.0000000000        1.4287085914        1.6153143456
H          0.8866543291       -0.5335571074        1.4336988265
H         -0.8965823230       -0.5141698905        1.4349731052
N          0.0994951518        1.4071527244        3.0719350326
C         -1.2838250345        2.1400610559        1.1622757420
H          0.8634228266        1.9671393514        1.2127098848
C         -0.4522561011        2.4131306259        3.8275924713
H          0.0559883156        0.4878883340        3.4868444047
N         -1.1028138592        3.1674931922        0.2898913881
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O         -2.3869915112        1.7218771704         1.4949014362
C         -0.7364233838        2.0603919868         5.2687517514
O         -0.6783709540        3.5220309504         3.3561347350
C         -2.2488097744        3.9887254309        -0.0692354283
H         -0.2071507663        3.6256369170         0.3378800427
H         -0.6356665397        2.9535387110         5.8787261494
H         -0.0766268483        1.2787024118         5.6423294220
H         -1.7673201561        1.7100197571         5.3352917316
H         -2.6304088314        4.5343080003         0.7953267143
H         -3.0397815968        3.3475089946        -0.4486505156
H         -1.9499838845        4.6891804832        -0.8450271228

AD: phi = -045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93837265, DF-LCCSD(T0)=-495.08478782
H          0.0000000000        0.0000000000         0.0000000000
C          0.0000000000        0.0000000000         1.0889241739
C          0.0000000000        1.4288243452         1.6156786137
H          0.8840326492       -0.5342060118         1.4372189106
H         -0.8971719452       -0.5165048581         1.4312436195
N          0.0683519046        1.4092306035         3.0696753130
C         -1.2743101921        2.1474980717         1.1509711950
H          0.8745481233        1.9655195759         1.2391623859
C         -0.2174917083        2.5573885877         3.7636148245
H         -0.2049377810        0.5440349323         3.5114694601
N         -1.0905924821        3.1055890687         0.2052147956
O         -2.3788557427        1.7970391022         1.5535645432
C         -0.5347462032        2.3758186424         5.2284895247
O         -0.2049187712        3.6541674616         3.2131398209
C         -2.2225107342        3.9223836775        -0.2037305921
H         -0.1798966329        3.5356262480         0.1912096914
H         -0.2023424445        3.2539925549         5.7747571978
H         -0.0731693509        1.4817315443         5.6443790797
H         -1.6172492594        2.2928868153         5.3336453410
H         -2.5748418598        4.5522108796         0.6145956724
H         -3.0365739274        3.2717508451        -0.5116181355
H         -1.9219357575        4.5448706047        -1.0426493604

AD: phi = -060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94021468, DF-LCCSD(T0)=-495.08629080
H          0.0000000000        0.0000000000         0.0000000000
C          0.0000000000        0.0000000000         1.0883663815
C          0.0000000000        1.4252871541         1.6103367175
H          0.8840942432       -0.5292396174         1.4421922453
H         -0.8998461517       -0.5183211050         1.4177667998
N          0.0790137200        1.4026669009         3.0733120411
C         -1.2575206582        2.1782981700         1.1373696003
H          0.8828816329        1.9604140698         1.2547245222
C          0.1429493804        2.5487314766         3.8132152307
H         -0.3452183896        0.6031391635         3.5205033111
N         -1.0751222284        3.4943674549         0.8733550401
O         -2.3334773267        1.5990483416         0.9913371965
C         -0.1284740761        2.3905853496         5.2914325025
O          0.4315599507        3.6370408614         3.3153209949
C         -2.2260887655        4.3260271671         0.5635552993
H         -0.2837930461        3.9191233775         1.3384617173
H          0.5705340391        3.0133937051         5.8435176242
H         -0.0484369586        1.3584492832         5.6269482904
H         -1.1368601155        2.7510513565         5.4957157847
H         -2.9000057303        4.4158235051         1.4172959478
H         -2.7792434644        3.8813095251        -0.2597339324
H         -1.8753168057        5.3125537599         0.2725747666
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AD: phi = -075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94269815, DF-LCCSD(T0)=-495.08840631
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0878773453
C          0.0000000000        1.4249473101        1.6095733612
H          0.8825698433       -0.5293867310        1.4450263867
H         -0.8999786964       -0.5216536524        1.4118401571
N          0.0361039119        1.4090363766        3.0721018611
C         -1.2343804096        2.1989195945        1.1085897396
H          0.8973661018        1.9561326674        1.2859240589
C          0.3906544918        2.4891754781        3.8168232879
H         -0.4134657624        0.6357902574        3.5370350987
N         -1.1118341347        3.5444673946        1.1680901596
O         -2.2390518459        1.6252709650        0.6899294733
C          0.2679200728        2.3288337133        5.3143111691
O          0.8086981215        3.5330144805        3.3092718501
C         -2.2465191680        4.3945641222        0.8546788921
H         -0.3356528748        3.9075916446        1.7088756216
H          1.2232353592        2.5854019484        5.7675106603
H         -0.0189600884        1.3234566418        5.6158219891
H         -0.4736603635        3.0390812112        5.6771841004
H         -3.0590018380        4.2586985700        1.5700829596
H         -2.6251850245        4.1507097766       -0.1354723345
H         -1.9193077317        5.4306950602        0.8709389965

AD: phi = -090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94281154, DF-LCCSD(T0)=-495.08851854
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0880236975
C          0.0000000000        1.4257115530        1.6087762113
H          0.8827694955       -0.5296571002        1.4444490506
H         -0.8993516090       -0.5228685780        1.4117463418
N          0.0091917218        1.4259629430        3.0700048861
C         -1.2332362214        2.2001470610        1.1144050547
H          0.8996748134        1.9589131371        1.2973407276
C          0.6264738049        2.3992654300        3.7881920305
H         -0.3987588075        0.6402897592        3.5504347143
N         -1.1136500909        3.5418948931        1.2494183615
O         -2.2287723555        1.6431069101        0.6573759828
C          0.6695771747        2.1982884562        5.2848019203
O          1.1167584406        3.3955644202        3.2503036370
C         -2.2343239688        4.4199575605        0.9675028830
H         -0.3100552284        3.8842571128        1.7618020782
H          0.1928679832        3.0513901840        5.7638140549
H          1.7122007220        2.1817244078        5.5977572695
H          0.1816170445        1.2810680763        5.6083200675
H         -3.0152978339        4.3317223287        1.7244158083
H         -2.6656408065        4.1586840034        0.0039371187
H         -1.8766948757        5.4457755018        0.9372227050

AD: phi = -105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94071072, DF-LCCSD(T0)=-495.08659403
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0885680922
C          0.0000000000        1.4259330110        1.6113496887
H          0.8830236550       -0.5291577688        1.4447949631
H         -0.8983605723       -0.5240381777        1.4133766566
N         -0.0096298882        1.4393759297        3.0714767791
C         -1.2299365266        2.2010136725        1.1216371462
H          0.9034984773        1.9576319309        1.3115973030
C          0.8388368498        2.2332244523        3.7823437374
H         -0.4967548060        0.6963395850        3.5467492727
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N         -1.0796244295        3.5458538293        1.2156351480
O         -2.2506591855        1.6538269713        0.7140743872
C          0.9043031883        1.9705877823        5.2690903541
O          1.4933169980        3.1287440115        3.2471692539
C         -2.1937303502        4.4433260515        0.9693046470
H         -0.2516208220        3.8875168111        1.6834065646
H          0.6931583770        2.8983589931        5.7968336374
H          1.9210050828        1.6704656728        5.5184633424
H          0.2112364032        1.1988101975        5.5983539908
H         -2.9215805498        4.4151841494        1.7817993076
H         -2.6961371789        4.1463725905        0.0519584940
H         -1.8134862627        5.4557417660        0.8611602776

AD: phi = -120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93970332, DF-LCCSD(T0)=-495.08561676
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904664502
C          0.0000000000        1.4302608802        1.6355637118
H          0.8869070701       -0.5234292363        1.4440818745
H         -0.8866226713       -0.5300339030        1.4383895052
N          0.0036319875        1.4440926715        3.0846097293
C         -1.2508083479        2.1623291614        1.1565086545
H          0.9039168440        1.9530327361        1.3191291173
C          1.0207223735        2.0248608515        3.7892548133
H         -0.9032867893        1.3560659721        3.5202241445
N         -1.1225143130        2.8518602478       -0.0014081496
O         -2.3171756264        2.0738136413        1.7639178772
C          0.7870653523        2.1440509070        5.2790824933
O          2.0681775253        2.3929987882        3.2639782525
C         -2.2534474879        3.5600768051       -0.5776186522
H         -0.2017635671        2.9887724512       -0.3812919101
H          1.5271247044        1.5338614106        5.7943293051
H         -0.2100101770        1.8308794377        5.5822021392
H          0.9494010900        3.1797932021        5.5708785952
H         -2.5493631644        4.4042608992        0.0447854706
H         -3.1019072050        2.8847848940       -0.6623658960
H         -1.9754510060        3.9176598738       -1.5653416998

AD: phi = -135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94034780, DF-LCCSD(T0)=-495.08621977
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904514443
C          0.0000000000        1.4292574185        1.6419316569
H          0.8909205440       -0.5177801914        1.4424825864
H         -0.8829695855       -0.5342610482        1.4411495170
N          0.0321936881        1.4419362418        3.0887572307
C         -1.2594300899        2.1695036180        1.2002032724
H          0.8943937407        1.9522607606        1.2959995123
C          1.1781366027        1.7344736215        3.7679650407
H         -0.8650068902        1.5426346577        3.5421391462
N         -1.2196501488        2.6991957065       -0.0445710388
O         -2.2612552966        2.2269336127        1.9126581884
C          1.0249320243        1.8821695589        5.2656252919
O          2.2681191130        1.8376240723        3.2094860790
C         -2.3694823609        3.3974391888       -0.5951804059
H         -0.3427917590        2.7157110411       -0.5359806689
H          1.5589182069        1.0657772658        5.7497351443
H         -0.0134065311        1.8726729246        5.5912298254
H          1.4963957441        2.8142940997        5.5699759951
H         -2.5878668945        4.3012659441       -0.0273055890
H         -3.2451577419        2.7527280254       -0.5604321519
H         -2.1555339392        3.6607268565       -1.6274302222
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AD: phi = -150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94099075, DF-LCCSD(T0)=-495.08681334
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904144374
C          0.0000000000        1.4293852944        1.6443593606
H          0.8930547518       -0.5141342028        1.4417177785
H         -0.8829299421       -0.5339479169        1.4418129137
N          0.0555884957        1.4385851633        3.0883970362
C         -1.2726134828        2.1662396179        1.2349173984
H          0.8812911390        1.9572279782        1.2706627126
C          1.2453703798        1.4329456673        3.7480837112
H         -0.8102497543        1.6508234464        3.5632928236
N         -1.3073872690        2.6003781388       -0.0461470902
O         -2.2200458278        2.3105950125        2.0070626458
C          1.1580178091        1.5447186819        5.2540532842
O          2.3195969732        1.3205772967        3.1597516450
C         -2.4754651185        3.2905770272       -0.5676088550
H         -0.4707583209        2.5445092759       -0.6005773582
H          1.5396556210        0.6233275277        5.6912749521
H          0.1443890760        1.7175387080        5.6103599268
H          1.8035946119        2.3584280867        5.5783857775
H         -2.6496891972        4.2224944926       -0.0310699888
H         -3.3582956592        2.6638309845       -0.4585381717
H         -2.3122075959        3.5034211616       -1.6205008549

AD: phi = -165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94085741, DF-LCCSD(T0)=-495.08660800
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904661219
C          0.0000000000        1.4318839370        1.6416606066
H          0.8920631942       -0.5145405847        1.4419142375
H         -0.8861583618       -0.5290688176        1.4413152369
N          0.0527614741        1.4480761243        3.0857088738
C         -1.2859576473        2.1481003216        1.2347868703
H          0.8731647940        1.9654670596        1.2572639454
C          1.1976710464        1.1647029462        3.7597406715
H         -0.8142887866        1.6528182060        3.5609539739
N         -1.3069029255        2.5943798201       -0.0446383927
O         -2.2354756950        2.2578504436        2.0088315525
C          1.0927834967        1.1884180622        5.2686549432
O          2.2523288241        0.9100379445        3.1793738097
C         -2.4733746406        3.2275418251       -0.6338254815
H         -0.4661580421        2.5052356555       -0.5897499119
H          1.8145896815        1.9060977612        5.6541914667
H          1.3665096241        0.2056884205        5.6488030278
H          0.0973800794        1.4486942993        5.6230930742
H         -2.3280307082        4.3018265570       -0.7449584838
H         -3.3140299293        3.0542351016        0.0318938599
H         -2.6866215885        2.7908362378       -1.6076794587

AD: phi = -180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93932883, DF-LCCSD(T0)=-495.08516452
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0904616604
C          0.0000000000        1.4217780976        1.6694154671
H          0.8658483571       -0.5445738132        1.4571536740
H         -0.9054828904       -0.5132959003        1.4176124650
N         -0.2420202032        1.4254578510        3.0968618313
C         -1.1156814726        2.2537722865        1.0379122530
H          0.9675208496        1.8918550038        1.4712029756
C          0.5691746732        0.7733223948        3.9737162332
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H          -1.1739311594         1.7076002042          3.3686358503
N          -0.8362941546         2.7256025854         -0.2016408867
O          -2.1882280130         2.4367587818          1.6110649312
C           0.0610945756         0.6996432671          5.3974791066
O           1.6518133387         0.2950490575          3.6403245154
C          -1.8019947638         3.4595752759         -0.9993996619
H           0.0795000697         2.5469317390         -0.5779581508
H           0.8432088847         1.0582389299          6.0633286727
H          -0.1298652628        -0.3448151736          5.6408926238
H          -0.8475108130         1.2769932778          5.5566907546
H          -1.4462487135         4.4672775144         -1.2098560106
H          -2.7215345633         3.5203077432         -0.4243726748
H          -1.9993415538         2.9443625221         -1.9385927404
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6.8 ψ profile for AD

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AD: psi = +000 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93851049, DF-LCCSD(T0)=-495.08440285
H           0.0000000000         0.0000000000          0.0000000000
C           0.0000000000         0.0000000000          1.0870177269
C           0.0000000000         1.4395374207          1.5911442848
H           0.8806558914        -0.5298187915          1.4484004826
H          -0.8948825654        -0.5250549868          1.4277639690
N          -0.0486293673         1.4580903051          3.0462004894
C          -1.1303713515         2.2209908647          0.9091317548
H           0.9198872853         1.9451072430          1.2901696545
C           0.6009785239         2.4160463361          3.7808387012
H          -0.3480566618         0.6195314750          3.5172959341
N          -2.0268420877         2.8270078815          1.7215401318
O          -1.1992123306         2.2587858916         -0.3167305579
C           0.6504821882         2.1731623627          5.2740464532
O           1.0965499346         3.4083171844          3.2599915500
C          -3.0525764892         3.6926063076          1.1679454965
H          -1.8145263325         2.8632404621          2.7036813483
H           0.3208644768         3.0750634544          5.7852371379
H           1.6866508069         1.9921065035          5.5571135293
H           0.0411949213         1.3293796931          5.5931411756
H          -3.7857568947         3.9094534768          1.9405327968
H          -3.5388801149         3.1853291037          0.3384169249
H          -2.6285327824         4.6262169319          0.7964101923

AD: psi = +015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93850381, DF-LCCSD(T0)=-495.08453806
H           0.0000000000         0.0000000000          0.0000000000
C           0.0000000000         0.0000000000          1.0861534543
C           0.0000000000         1.4353726586          1.5964905448
H           0.8790716645        -0.5304907202          1.4504864737
H          -0.8972720656        -0.5233840206          1.4223010584
N          -0.0264049111         1.4271108149          3.0531772481
C          -1.1328609141         2.2312612262          0.9240569722
H           0.9226652801         1.9392114171          1.2937974574
C           0.4493574341         2.4432044183          3.8233581976
H          -0.3050058066         0.5729878055          3.5078792858
N          -1.8352471797         3.0834560976          1.7113293304
O          -1.3763843045         2.0664006319         -0.2687299262
C           0.5322734317         2.1636205717          5.3074877279
O           0.7839643446         3.5239160164          3.3387917030
C          -2.8027180746         3.9771098824          1.0941587007
H          -1.3805737451         3.3918547075          2.5566317897
H           0.1059687236         3.0061930892          5.8470558944
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H          1.5838943457        2.0897505163        5.5826442581
H          0.0244161710        1.2462799862        5.5995973884
H         -3.3413679865        4.5026731916        1.8783856014
H         -3.5036325231        3.3924538757        0.5040586057
H         -2.3207871134        4.6994540784        0.4335964324

AD: psi = +030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94003123, DF-LCCSD(T0)=-495.08594012
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0859007405
C          0.0000000000        1.4311622850        1.6011762989
H          0.8786452471       -0.5306481748        1.4508431028
H         -0.8990802611       -0.5234590095        1.4152811338
N         -0.0117033149        1.4154115822        3.0610068840
C         -1.1454538017        2.2379585020        0.9570570691
H          0.9235779135        1.9365180573        1.3003292370
C          0.4410611135        2.4255563064        3.8444824023
H         -0.3058877472        0.5623869695        3.5081412223
N         -1.6094398423        3.2902871757        1.6744520449
O         -1.6043887936        1.9154676386       -0.1364788431
C          0.5066423726        2.1379655409        5.3267984836
O          0.7778652157        3.5162175711        3.3765986476
C         -2.5838927529        4.1813633187        1.0648170071
H         -0.9834451268        3.6651242195        2.3762629660
H         -0.0002921885        2.9394167094        5.8597386946
H          1.5528166286        2.1470911607        5.6298533801
H          0.0646119893        1.1815901313        5.5990142590
H         -2.8703965756        4.9330480593        1.7955541844
H         -3.4623474912        3.6126983015        0.7694616298
H         -2.1823400567        4.6698463034        0.1757580928

AD: psi = +045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94159009, DF-LCCSD(T0)=-495.08734377
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0864101004
C          0.0000000000        1.4276874827        1.6051780056
H          0.8794691559       -0.5302744121        1.4500167719
H         -0.8997423644       -0.5246909990        1.4102203723
N         -0.0065792795        1.4147716467        3.0658634097
C         -1.1669293727        2.2344428492        0.9994617673
H          0.9202280305        1.9397135223        1.3067081668
C          0.4899282879        2.4103906762        3.8401550110
H         -0.3601461608        0.5874321039        3.5187450056
N         -1.3946491212        3.4340776120        1.5805157173
O         -1.8352314690        1.7997437821        0.0631885590
C          0.5210987534        2.1421344575        5.3268532689
O          0.8968470987        3.4733312982        3.3621779605
C         -2.4065705998        4.3223122320        1.0368537984
H         -0.6799671424        3.7945855602        2.2017836549
H          0.0393767495        2.9717337511        5.8400396559
H          1.5616171220        2.1119160883        5.6471370713
H          0.0343128783        1.2093440123        5.6049114512
H         -2.4814930655        5.1961921967        1.6786351974
H         -3.3677982161        3.8133845793        1.0065805428
H         -2.1591659794        4.6367294376        0.0220676581

AD: psi = +060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94264449, DF-LCCSD(T0)=-495.08829425
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0871108002
C          0.0000000000        1.4258215155        1.6082948721
H          0.8809424653       -0.5298507142        1.4477150969
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H          -0.8999315776       -0.5240625494        1.4090268728
N           0.0119698118        1.4148810456        3.0693930411
C          -1.2056905713        2.2157512157        1.0613266990
H           0.9082705347        1.9500754324        1.3002767375
C           0.5224707165        2.4214627613        3.8213960441
H          -0.3908163956        0.6178172566        3.5355183173
N          -1.2405064571        3.5113537723        1.4411817841
O          -2.0634012179        1.6961183784        0.3490380826
C           0.5105813991        2.2058760428        5.3167299529
O           0.9698979067        3.4560467305        3.3181068343
C          -2.3232994957        4.3770205953        1.0125792028
H          -0.4742556403        3.8653813023        2.0008539248
H          -0.0844264496        2.9939496389        5.7750977635
H           1.5301576610        2.3031066817        5.6851740526
H           0.1119786895        1.2361024670        5.6078845971
H          -2.1401079038        5.3767762304        1.3969933781
H          -3.2793856069        4.0147459411        1.3894028288
H          -2.3816557676        4.4117397162       -0.0747512383

AD: psi = +075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94308720, DF-LCCSD(T0)=-495.08875918
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0879247287
C           0.0000000000        1.4255257875        1.6085954953
H           0.8825536485       -0.5296828826        1.4448428749
H          -0.8997447458       -0.5223431792        1.4114435778
N           0.0177282705        1.4194580752        3.0699169611
C          -1.2317183506        2.2008577358        1.1062969882
H           0.8999219011        1.9570772225        1.2936021069
C           0.5193902154        2.4479749233        3.8005257826
H          -0.4043543961        0.6389551717        3.5468752336
N          -1.1195540009        3.5433744818        1.2269796672
O          -2.2239093124        1.6375099757        0.6477672941
C           0.4999840942        2.2693998290        5.3006458854
O           0.9741548777        3.4669115757        3.2734285642
C          -2.2455729928        4.4068583319        0.9208244903
H          -0.3295347702        3.8949018166        1.7547685032
H          -0.0497407233        3.0990460201        5.7411710995
H           1.5246596067        2.3191551698        5.6651039988
H           0.0513452275        1.3291302433        5.6148523459
H          -3.0672732954        4.2568441929        1.6226250815
H          -2.6130510471        4.1905986885       -0.0800288634
H          -1.9143151853        5.4407694561        0.9681735524

AD: psi = +090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94257965, DF-LCCSD(T0)=-495.08840080
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0886450518
C           0.0000000000        1.4260341311        1.6103097667
H           0.8833973037       -0.5297197671        1.4431507968
H          -0.8993503264       -0.5201959435        1.4164074553
N           0.0410091604        1.4222350819        3.0693822257
C          -1.2578160012        2.1796228381        1.1498110594
H           0.8875801487        1.9647687734        1.2774637948
C           0.4910562229        2.4991592908        3.7684957295
H          -0.4348760108        0.6810655288        3.5587049683
N          -1.0683700726        3.5097035750        0.9694159993
O          -2.3316063457        1.6106187288        0.9647633387
C           0.4267185285        2.3876029710        5.2739062498
O           0.9376840609        3.5022251244        3.2077611471
C          -2.2027207310        4.3744310710        0.6923211992
H          -0.2405936639        3.9006113678        1.4010331145
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H          1.4245658064        2.5556969236        5.6745244751
H          0.0572242128        1.4228823801        5.6158254282
H         -0.2205403496        3.1773790146        5.6517740322
H         -2.8846278034        4.4305452928        1.5423823938
H         -2.7540336049        3.9825085500       -0.1589249411
H         -1.8342333669        5.3692935824        0.4567590882

AD: psi = +105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94142068, DF-LCCSD(T0)=-495.08742642
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0890959497
C          0.0000000000        1.4273103177        1.6126792149
H          0.8835008820       -0.5303823180        1.4422561723
H         -0.8987606105       -0.5184742366        1.4218720627
N          0.0485174836        1.4221085883        3.0685919353
C         -1.2686063095        2.1614258307        1.1578157440
H          0.8834769074        1.9665282427        1.2714547107
C          0.4280298823        2.5419079876        3.7476281056
H         -0.4550656037        0.6994608553        3.5582491880
N         -1.0551088247        3.4091376487        0.6690213660
O         -2.3762644421        1.6322607654        1.2168741926
C          0.3259492204        2.4704712373        5.2535681584
O          0.8438657381        3.5445895011        3.1663192255
C         -2.1878361165        4.2585895092        0.3387551444
H         -0.1915301078        3.8467986578        0.9570918285
H          1.2914039423        2.7379280668        5.6782875090
H          0.0303586200        1.4874050815        5.6145570078
H         -0.4006650720        3.2104141372        5.5858906424
H         -2.7524181730        4.5420960003        1.2283588625
H         -2.8538802127        3.7187632367       -0.3294405031
H         -1.8220426462        5.1522066932       -0.1599840172

AD: psi = +120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94040428, DF-LCCSD(T0)=-495.08656802
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0893279344
C          0.0000000000        1.4286107874        1.6160271082
H          0.8827447880       -0.5317521784        1.4422416387
H         -0.8978327254       -0.5184295516        1.4261613896
N          0.0427543105        1.4180330130        3.0689994603
C         -1.2685686538        2.1496253352        1.1461133360
H          0.8853004928        1.9651671871        1.2748768107
C          0.3274759930        2.5736271236        3.7411427548
H         -0.4978632341        0.7111537658        3.5430262447
N         -1.0579533123        3.2469450240        0.3757188050
O         -2.3850803769        1.7145566196        1.4177183666
C          0.1550599974        2.5237663018        5.2415124826
O          0.7154878263        3.5833800871        3.1565055209
C         -2.1848325372        4.0671625725       -0.0381707559
H         -0.1573705703        3.6888179025        0.4766841860
H          1.0518404978        2.9256327308        5.7078950820
H         -0.0309424600        1.5182264858        5.6136173171
H         -0.6807646579        3.1673694311        5.5134210856
H         -2.6480524445        4.5717865621        0.8108757525
H         -2.9319225871        3.4324075865       -0.5075021186
H         -1.8365712660        4.8057739601       -0.7553990334

AD: psi = +135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94004708, DF-LCCSD(T0)=-495.08580626
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0908854500
C          0.0000000000        1.4311383116        1.6338499670
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H          0.8926778888       -0.5150168817        1.4418364581
H         -0.8871940263       -0.5254524512        1.4426934945
N          0.0365682255        1.4629588208        3.0828915020
C         -1.2738831046        2.1519375692        1.2100570141
H          0.8885665273        1.9556870481        1.2779980256
C          1.2056628457        1.3215516781        3.7652038647
H         -0.8524826892        1.4496174274        3.5595595583
N         -1.1314162629        3.0330430149        0.1895618246
O         -2.3437999738        1.9204355551        1.7707747725
C          1.0843115386        1.2959376779        5.2727774413
O          2.2905683614        1.2340608630        3.1932971557
C         -2.2519187752        3.7611819109       -0.3782885656
H         -0.2068769824        3.1828213983       -0.1769738614
H          1.6947433936        2.0987655072        5.6820540600
H          1.4898220431        0.3528885254        5.6352727990
H          0.0593306215        1.4070023380        5.6211300937
H         -2.1500338286        4.8314333098       -0.2029533145
H         -3.1538070740        3.4057126498        0.1119450645
H         -2.3266418055        3.5774792440       -1.4489510012

AD: psi = +150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94075009, DF-LCCSD(T0)=-495.08649193
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0906899960
C          0.0000000000        1.4317682258        1.6385776848
H          0.8927839089       -0.5140103260        1.4422766838
H         -0.8855957168       -0.5285376349        1.4430439363
N          0.0435688946        1.4541588351        3.0841312041
C         -1.2780336356        2.1498337211        1.2182101023
H          0.8822112713        1.9594439041        1.2690496062
C          1.2074801312        1.2716944987        3.7619524420
H         -0.8394051059        1.5668742685        3.5597524586
N         -1.2118764267        2.7811432017        0.0203979144
O         -2.2903021558        2.1112209997        1.9156757710
C          1.0970381531        1.2902112008        5.2704537735
O          2.2809873980        1.1056690412        3.1846131217
C         -2.3568631313        3.4379419079       -0.5845330149
H         -0.3264699776        2.7930827315       -0.4569476786
H          1.7614255195        2.0611499337        5.6562819917
H          1.4432763421        0.3316836842        5.6533352360
H          0.0838874399        1.4750940844        5.6220264144
H         -2.1987704699        4.5134906985       -0.6537046965
H         -3.2164555936        3.2465724462        0.0514398482
H         -2.5477058821        3.0376666607       -1.5790640192

AD: psi = +165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94112910, DF-LCCSD(T0)=-495.08692707
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0903801824
C          0.0000000000        1.4294790843        1.6456515048
H          0.8929996474       -0.5137734436        1.4412755391
H         -0.8841387940       -0.5325500255        1.4410789445
N          0.0611591039        1.4359583064        3.0892296425
C         -1.2805512556        2.1601873331        1.2485968009
H          0.8740778415        1.9622994474        1.2611559790
C          1.2382853099        1.2674201286        3.7470432894
H         -0.7899110817        1.6920888158        3.5691160249
N         -1.3586923552        2.5332851770       -0.0494123933
O         -2.1985042654        2.3516633923        2.0458247110
C          1.1654851397        1.3595630540        5.2551153100
O          2.2936573445        1.0507354945        3.1528919670
C         -2.5397587215        3.2082282522       -0.5613365529
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H          -0.5502196550        2.4251357926       -0.6367640705
H           1.8209501337        2.1642615711        5.5837252721
H           1.5438897098        0.4302507948        5.6769852725
H           0.1573039341        1.5399981087        5.6228290596
H          -2.6861949757        4.1668186259       -0.0650754192
H          -3.4234445008        2.5967399548       -0.3899849288
H          -2.4132225304        3.3683660504       -1.6285107447

AD: psi = -015 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93842381, DF-LCCSD(T0)=-495.08436506
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0874829608
C           0.0000000000        1.4398807674        1.5917036067
H           0.8837431233       -0.5303891679        1.4423670160
H          -0.8926774414       -0.5259336061        1.4317237544
N          -0.0286420284        1.4508065606        3.0470724545
C          -1.1585408327        2.1981974312        0.9349648950
H           0.9021460133        1.9572813118        1.2601681379
C           0.4351354071        2.5272602832        3.7596144741
H          -0.1310290520        0.5703893294        3.5258374897
N          -2.2104042067        2.5050536188        1.7312437089
O          -1.1306888171        2.4347066502       -0.2691665605
C           0.5576796917        2.3217236684        5.2540842862
O           0.7184259311        3.5863006541        3.2135789481
C          -3.3060478918        3.3073098210        1.2166878153
H          -2.0714163424        2.4285324092        2.7245442138
H           0.0912264915        3.1635607348        5.7609576981
H           1.6153143135        2.3220072183        5.5151781699
H           0.1064438874        1.3925606063        5.5979131112
H          -4.1197502522        3.2959453029        1.9373603296
H          -3.6494286649        2.8829176353        0.2765175591
H          -2.9951568396        4.3367123792        1.0340804541

AD: psi = -030 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93839570, DF-LCCSD(T0)=-495.08421823
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0889507979
C           0.0000000000        1.4492240575        1.5864608359
H           0.8910899350       -0.5172420066        1.4435623703
H          -0.8805951682       -0.5280414733        1.4483381347
N           0.0735087256        1.5297617393        3.0486670867
C          -1.1476705286        2.2179900243        0.9147213751
H           0.8983980602        1.9443434067        1.2199922159
C          -0.7682266489        0.9520665077        3.9426948433
H           0.8747887582        2.0045988256        3.4286259627
N          -2.2937402962        2.3698479457        1.6148970465
O          -0.9793152012        2.6637913678       -0.2198220914
C          -0.3464471716        1.0419977567        5.3924973169
O          -1.8148810941        0.3875629735        3.6129913210
C          -3.4435743399        2.9797126326        0.9676027891
H          -2.4361595009        1.7418354932        2.3979919699
H          -1.1901311769        1.4019078993        5.9770219262
H           0.5131535653        1.6893370383        5.5541088775
H          -0.1056246190        0.0377034793        5.7391434902
H          -3.7829708848        2.3900987264        0.1148687405
H          -3.1781618194        3.9710087526        0.6072980364
H          -4.2463487918        3.0629700736        1.6953569987

AD: psi = -045 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93914054, DF-LCCSD(T0)=-495.08487117
H           0.0000000000        0.0000000000        0.0000000000
C           0.0000000000        0.0000000000        1.0895483741
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C          0.0000000000        1.4483847269        1.5852491353
H          0.8935768881       -0.5154756470        1.4409013625
H         -0.8772987419       -0.5335626281        1.4470283246
N          0.0914293313        1.5400660027        3.0466771920
C         -1.1625294909        2.2267313319        0.9498797437
H          0.8895899715        1.9489879021        1.2057622641
C         -0.7187682753        0.9401697456        3.9548675998
H          0.8620709116        2.0725831900        3.4133664293
N         -2.3668955095        2.1105712873        1.5459285637
O         -0.9690373640        2.8889861577       -0.0701847666
C         -0.3030181913        1.0882312329        5.4015571938
O         -1.7321967849        0.3082412805        3.6427177477
C         -3.5349487928        2.7377579414        0.9547008311
H         -2.4615813547        1.4361460641        2.2974068355
H         -1.1558480061        1.4519516526        5.9706890698
H          0.5426196008        1.7582524278        5.5433318112
H         -0.0445814414        0.1016430132        5.7839055225
H         -3.7517879692        2.3209453880       -0.0293446011
H         -3.3674070961        3.8068498502        0.8374039992
H         -4.3847735949        2.5752092433        1.6122884973

AD: psi = -060 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93918186, DF-LCCSD(T0)=-495.08494204
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898094700
C          0.0000000000        1.4459830575        1.5866960055
H          0.8964901891       -0.5119787178        1.4392438307
H         -0.8732001062       -0.5407020853        1.4444835958
N          0.0935915534        1.5409253949        3.0489876938
C         -1.1615588804        2.2572341488        0.9899797156
H          0.8887085935        1.9486448408        1.2080463241
C         -0.7260500630        0.9415174343        3.9497320583
H          0.8425537883        2.1020887511        3.4178230496
N         -2.3976226652        1.9191031181        1.4100498666
O         -0.9457894922        3.1286150596        0.1462879593
C         -0.3453942910        1.1210286242        5.4025567229
O         -1.7194675772        0.2839959229        3.6268939361
C         -3.5618541621        2.6236654755        0.9060152359
H         -2.4785628181        1.2223746122        2.1422427852
H         -1.2038769039        1.5223953695        5.9372457476
H          0.5122982956        1.7744689639        5.5485639265
H         -0.1232898848        0.1399775081        5.8197557312
H         -4.4496542207        2.1964102961        1.3644407980
H         -3.6292264483        2.5235035470       -0.1764281569
H         -3.5069161761        3.6861920412        1.1424908521

AD: psi = -075 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93857459, DF-LCCSD(T0)=-495.08451746
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0898901639
C          0.0000000000        1.4435377934        1.5880190761
H          0.8997199480       -0.5073385244        1.4381796288
H         -0.8680741634       -0.5494521853        1.4420283396
N          0.0721141801        1.5415676027        3.0505937385
C         -1.1439169628        2.2987324792        1.0163825836
H          0.8979769388        1.9410882861        1.2237588876
C         -0.8012875708        0.9714197816        3.9209406920
H          0.7912264778        2.1298171810        3.4362085195
N         -2.3897787972        1.8021195042        1.1873382636
O         -0.9047393437        3.3415598480        0.4070525054
C         -0.4983688654        1.1842035178        5.3872399500
O         -1.7785683994        0.3112296609        3.5585163067
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C         -3.5430153918        2.5745078257        0.7600644722
H         -2.4962229030        1.0733296930        1.8839701209
H         -1.3797255091        1.6096090516        5.8630635253
H          0.3580540804        1.8321779318        5.5626232229
H         -0.3115990326        0.2126409136        5.8420785535
H         -4.4373918194        1.9769956124        0.9156083973
H         -3.4504199077        2.8180877973       -0.2961099101
H         -3.6288332687        3.5094171268        1.3158871143

AD: psi = -090 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93725905, DF-LCCSD(T0)=-495.08347252
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0896095660
C          0.0000000000        1.4394153126        1.5955051457
H          0.9013567860       -0.5040479202        1.4383262839
H         -0.8624229162       -0.5579808243        1.4423062553
N          0.0665579787        1.5263916270        3.0577487785
C         -1.1332931236        2.3336999488        1.0613289090
H          0.9021997725        1.9359984350        1.2390774404
C         -0.8754112343        1.0072789569        3.8908783654
H          0.7632811255        2.1320739072        3.4571826015
N         -2.3499637437        1.7480910742        0.9454188266
O         -0.9030097119        3.4944952264        0.7247880058
C         -0.6430811843        1.2362017281        5.3677789858
O         -1.8502022782        0.3731060834        3.4827240532
C         -3.4964312991        2.5585387724        0.5676440963
H         -2.5016335198        0.9448751666        1.5419395966
H         -1.5299374443        1.7073907579        5.7870343718
H          0.2291014571        1.8523349360        5.5769087982
H         -0.5216566008        0.2674897397        5.8498361800
H         -4.3542047647        1.9053903281        0.4303500792
H         -3.2805776246        3.0725011170       -0.3657094086
H         -3.7275441427        3.3106362334        1.3238705138

AD: psi = -105 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93595359, DF-LCCSD(T0)=-495.08239201
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0894546555
C          0.0000000000        1.4348495768        1.6076701223
H          0.9005178812       -0.5051273211        1.4378436764
H         -0.8597279536       -0.5608611554        1.4471564579
N          0.0297687429        1.4960259131        3.0699733020
C         -1.1110431087        2.3620558467        1.0805361924
H          0.9170384805        1.9249578753        1.2792608973
C         -1.0121494945        1.0644676343        3.8364241088
H          0.6947195733        2.1193877480        3.4963229999
N         -2.2419397574        1.7649072226        0.6300350268
O         -0.9271167123        3.5772840004        1.0455545519
C         -0.8938997855        1.3392728574        5.3188533552
O         -1.9863703443        0.4840011704        3.3584215440
C         -3.3797657827        2.5915353593        0.2593390629
H         -2.4323052243        0.8544406929        1.0210278233
H         -1.0781750520        0.4124887260        5.8579959961
H         -1.6716288212        2.0487092825        5.5987127033
H          0.0767301915        1.7394679654        5.6048971216
H         -4.1392766932        1.9585678603       -0.1921951374
H         -3.0564856311        3.3384038288       -0.4608851574
H         -3.8007551627        3.1087983867        1.1231353221

AD: psi = -120 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93561837, DF-LCCSD(T0)=-495.08214367
H          0.0000000000        0.0000000000        0.0000000000
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C          0.0000000000        0.0000000000        1.0898278163
C          0.0000000000        1.4300482054        1.6217641098
H          0.8988784404       -0.5100027997        1.4338184234
H         -0.8614857256       -0.5562938657        1.4545712071
N          0.0311971679        1.4608025432        3.0825444161
C         -1.1263439303        2.3570845758        1.1255142498
H          0.9152018834        1.9266799254        1.2952869399
C         -1.0773760354        1.1301264716        3.8099352963
H          0.6950354133        2.0800560055        3.5173858744
N         -2.1132935886        1.7934802531        0.3865981487
O         -1.0735681930        3.5597096172        1.3709293776
C         -1.0042613252        1.4340923426        5.2889181112
O         -2.0682414704        0.6205689426        3.2913823271
C         -3.2761805844        2.5923600334        0.0338679825
H         -2.2476635181        0.8032091686        0.5088375753
H         -1.4224749251        0.5947641130        5.8390741981
H         -1.6220846790        2.3097781396        5.4875429071
H          0.0099167501        1.6297074581        5.6318577042
H         -3.9006137109        2.0202162319       -0.6474642049
H         -2.9462394408        3.5037559745       -0.4574793531
H         -3.8536080248        2.8678425611        0.9177658604

AD: psi = -135 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93696000, DF-LCCSD(T0)=-495.08302487
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0917368046
C          0.0000000000        1.4235472371        1.6416162746
H          0.9071053737       -0.5018200676        1.4191174937
H         -0.8617251104       -0.5577659364        1.4598975020
N          0.1176178455        1.4209406462        3.0948277988
C         -1.2520721725        2.2505296165        1.3300939883
H          0.8537884254        1.9652078967        1.2182716899
C          1.3293823855        1.1628465429        3.6792546854
H         -0.4898667518        2.0752903659        3.5690244373
N         -2.1098195394        1.7558201367        0.4110367490
O         -1.4716965420        3.3056355419        1.9261623945
C          1.3996275850        1.4222372428        5.1681409846
O          2.2849875557        0.7258553363        3.0449628740
C         -3.3040505184        2.4983555533        0.0447080546
H         -1.9083182416        0.8782927154       -0.0325653730
H          1.7107409274        0.5054502391        5.6651837203
H          0.4532566686        1.7575216500        5.5872936415
H          2.1650650752        2.1750879887        5.3499689845
H         -3.0387657713        3.4860959723       -0.3284564756
H         -3.9536806866        2.6253090122        0.9092409835
H         -3.8322588997        1.9474254824       -0.7286024935

AD: psi = -150 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93855342, DF-LCCSD(T0)=-495.08453897
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0917334224
C          0.0000000000        1.4216366886        1.6517268647
H          0.9108509070       -0.4993410468        1.4134536186
H         -0.8621765347       -0.5587536032        1.4556465359
N          0.1877182912        1.4146663987        3.0925974740
C         -1.2870093776        2.2140427184        1.3967329432
H          0.8236247902        1.9794680929        1.1900531402
C          1.4312374494        1.1994239891        3.6184794016
H         -0.4484766635        2.0136463266        3.6020712412
N         -2.0092089272        1.8714007683        0.3075540678
O         -1.6444206421        3.1131871114        2.1587596157
C          1.5538595230        1.4219302561        5.1097740816
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O          2.3773067025        0.8204923208        2.9327482904
C         -3.2183910380        2.6012784212       -0.0347807923
H         -1.7085555803        1.1031338154       -0.2639447029
H          1.8407821148        0.4815104129        5.5772898125
H          0.6328482220        1.7818499214        5.5636624156
H          2.3538247062        2.1384938566        5.2868042399
H         -2.9983871655        3.6587799960       -0.1702518817
H         -3.9594715595        2.5068295993        0.7574185947
H         -3.6204063373        2.1932166068       -0.9580428755

AD: psi = -165 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.93977283, DF-LCCSD(T0)=-495.08568591
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0911328883
C          0.0000000000        1.4198752001        1.6622957484
H          0.9073922875       -0.5033255521        1.4176967784
H         -0.8687301961       -0.5534562980        1.4466358369
N          0.1779785255        1.4011646762        3.0994151871
C         -1.2983747211        2.1893245639        1.3959876714
H          0.8267721404        1.9802565916        1.2105893859
C          1.4161938740        1.2097002236        3.6386406927
H         -0.5219226468        1.9117599103        3.6215192743
N         -1.8239878989        2.0633810489        0.1570486043
O         -1.8380296512        2.8740765411        2.2655484907
C          1.5080740790        1.3838212574        5.1384485262
O          2.3860761455        0.8883126224        2.9551996618
C         -3.0192009981        2.7998646259       -0.2185279917
H         -1.3510326261        1.4976129033       -0.5241138535
H          1.7952390060        0.4310260649        5.5803119634
H          0.5746302312        1.7193068568        5.5857471514
H          2.2970932462        2.1014541782        5.3550251801
H         -2.8534578669        3.8730521156       -0.1352874149
H         -3.8487828813        2.5317248257        0.4330672386
H         -3.2712991837        2.5507560867       -1.2456234897

AD: psi = -180 degree, Basis set = Aug-cc-pVTZ, energy in hartrees.
DF-LMP2=-494.94056951, DF-LCCSD(T0)=-495.08642596
H          0.0000000000        0.0000000000        0.0000000000
C          0.0000000000        0.0000000000        1.0905445450
C          0.0000000000        1.4343275802        1.6325166314
H          0.9066577834       -0.4991550820        1.4264576348
H         -0.8720883969       -0.5455815080        1.4496624725
N          0.2239171419        1.4696557684        3.0589888823
C         -1.3344432760        2.1382448271        1.3754531723
H          0.8023574954        1.9938253488        1.1402495035
C          1.4762158963        1.3335606712        3.5735213187
H         -0.5310650527        1.8523229864        3.6114820269
N         -1.7200822075        2.2062644152        0.0804598462
O         -2.0285829956        2.5841421145        2.2888958221
C          1.5909148173        1.5101251951        5.0714176578
O          2.4478753687        1.0679630617        2.8675928534
C         -2.9511588521        2.8826464923       -0.2928921314
H         -1.0883247118        1.8916586520       -0.6346970204
H          1.9883865213        0.5910686868        5.4985265583
H          0.6407211214        1.7467230386        5.5460498576
H          2.3064056447        2.3056521509        5.2717600236
H         -2.9211826932        3.9333146198       -0.0065943445
H         -3.7996582794        2.4176114010        0.2050251591
H         -3.0776119424        2.8034957696       -1.3691483769
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