

Comparative Conformational Analyses and Molecular Dynamics Studies of Glycylglycine Methyl Ester and Glycylglycine *N*-methylester

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Supporting Information

This document provides Cartesian coordinates (in Å) for the optimized geometries of *N*-methylacetamide (NMA), glycylglycine methyl ester (GGMe) and glycylglycine *N*-methylester (GGAm).

Each conformer is named as [Compound name]_[Trans/Cis]_[GP/WP]^a_[Conf_number]^b

1. NMA_trans_GP

C	-0.07680	1.02250	0.03930
N	-1.37820	1.67120	-0.03760
C	-2.53190	1.00130	0.25440
C	-3.81650	1.80890	0.16190
O	-2.53220	-0.18760	0.56570
H	0.66620	1.66030	-0.44410
H	0.22370	0.84330	1.07790
H	-0.11370	0.05810	-0.47290
H	-1.42140	2.65780	-0.24020
H	-4.48090	1.32800	-0.56140
H	-4.31690	1.78490	1.13410
H	-3.66260	2.85090	-0.13440

^aGP: Gas phase; WP: water phase (water dielectric continuum)

^bConf_Number: Conformer number; there is no conformer number for NMA geometries as there is only single conformer for trans and cis geometries each for NMA.

2. NMA_Cis_GP

C	-1.12120	2.95120	0.14880
N	-1.19680	1.49790	0.15460
C	-2.32990	0.72890	0.18670
C	-3.65450	1.47230	0.22120
O	-2.26400	-0.49830	0.18760
H	-0.11060	3.24500	0.43910
H	-1.32000	3.37050	-0.84450
H	-1.81960	3.40270	0.86310
H	-0.33820	0.96440	0.13230
H	-4.23120	1.18290	-0.65690
H	-4.22410	1.22660	1.12450
H	-3.50210	2.55730	0.21230

3. GGMe_Trans_GP_Conf_1:

N	9.04370	-4.93980	-0.01460
C	9.09650	-3.47660	0.04680
C	8.60670	-2.90640	1.38220
N	8.46310	-3.81050	2.37970
C	8.04500	-3.41410	3.70260
C	7.86440	-4.63610	4.57890
O	7.46080	-4.28470	5.81230
C	7.25790	-5.36570	6.74680
O	8.05990	-5.78170	4.22560
O	8.38670	-1.70240	1.51800
H	9.76360	-5.31940	-0.61950
H	8.14650	-5.27250	-0.35470
H	8.52870	-2.96240	-0.73960
H	10.13800	-3.15340	-0.05820
H	8.67530	-4.78530	2.18730
H	7.10380	-2.85210	3.66600
H	8.77570	-2.74380	4.17450
H	6.94580	-4.88830	7.67470
H	6.48330	-6.04280	6.37980
H	8.18710	-5.92190	6.89010

4. GGMe_Trans_GP_Conf_2

N	9.52520	-4.86590	0.12040
C	9.04260	-3.48520	0.03180
C	8.60660	-2.90630	1.38240
N	8.46310	-3.81080	2.37970
C	8.03370	-3.41750	3.69980
C	8.09370	-4.60370	4.63990
O	7.70510	-4.25190	5.87820
C	7.71310	-5.30130	6.86890
O	8.43940	-5.72490	4.32600
O	8.38670	-1.70230	1.51780
H	9.34640	-5.38500	-0.73220
H	10.52300	-4.90730	0.30470
H	8.15590	-3.45840	-0.61100
H	9.76080	-2.77370	-0.39590
H	8.66690	-4.78660	2.18300
H	7.00910	-3.02280	3.69140
H	8.66250	-2.60970	4.09360
H	7.03900	-6.10780	6.57170
H	8.72290	-5.69950	6.99040
H	7.37010	-4.83010	7.78900

5. GGMe_Trans_GP_Conf_3

N	9.06710	-4.94180	0.03620
C	8.97740	-3.47870	0.03950
C	8.76930	-2.88940	1.43910
N	8.37660	-3.78580	2.38160
C	8.21670	-3.42490	3.76640
C	8.98200	-4.36180	4.68730
O	8.85250	-3.96890	5.96880
C	9.51560	-4.78570	6.95590
O	9.60520	-5.34160	4.33460
O	8.92590	-1.68760	1.64930
H	8.76210	-5.33550	-0.84740
H	10.01630	-5.26160	0.20670
H	8.10860	-3.17530	-0.55490
H	9.84730	-2.96310	-0.38710
H	8.35980	-4.75990	2.09620
H	7.16280	-3.43340	4.07670
H	8.57610	-2.39940	3.89770
H	9.12730	-5.80640	6.92660
H	10.59220	-4.80250	6.77180
H	9.29530	-4.31570	7.91360

6. GGMe_Trans_GP_Conf_4

N	9.01900	-4.93740	-0.01620
C	9.10360	-3.47570	0.05330
C	8.60540	-2.90340	1.38520
N	8.46370	-3.81640	2.38050
C	7.94020	-3.46720	3.67580
C	6.84200	-4.42220	4.11430
O	6.33870	-4.04540	5.30530
C	5.29790	-4.88270	5.85000
O	6.47730	-5.40330	3.50050
O	8.38740	-1.69960	1.51420
H	8.11260	-5.24730	-0.35430
H	9.72770	-5.32770	-0.62760
H	8.55560	-2.94510	-0.73590
H	10.15320	-3.17520	-0.03680
H	8.60880	-4.78820	2.12540
H	7.54860	-2.44630	3.62480
H	8.71840	-3.46810	4.45170
H	4.43930	-4.90660	5.17510
H	5.66850	-5.89940	6.00010
H	5.02830	-4.42520	6.80110

7. GGMe_Trans_GP_Conf_5

N	9.54910	-2.52730	-0.93760
C	9.03660	-3.49560	0.01620
C	8.60950	-2.90670	1.37250
N	8.46140	-3.80590	2.38330
C	7.98680	-3.41150	3.69160
C	7.90740	-4.63240	4.58550
O	7.46860	-4.30880	5.81060
C	7.35170	-5.39660	6.75410
O	8.20280	-5.75990	4.23870
O	8.38570	-1.70680	1.52410
H	8.90350	-1.74270	-0.99700
H	10.42690	-2.13800	-0.60250
H	9.78350	-4.28360	0.16940
H	8.15440	-3.98680	-0.41660
H	8.65900	-4.79050	2.25110
H	6.99780	-2.94040	3.63380
H	8.65150	-2.66990	4.15160
H	6.64890	-6.14510	6.38180
H	8.32650	-5.86170	6.91600
H	6.98260	-4.94120	7.67180

8. GGMe_Trans_GP_Conf_6

N	8.92520	-2.62200	-1.11450
C	9.11450	-3.48480	0.03840
C	8.60940	-2.90670	1.37260
N	8.46140	-3.80590	2.38330
C	8.06680	-3.39940	3.71440
C	7.99010	-4.61990	4.60910
O	7.62570	-4.28590	5.85560
C	7.52020	-5.37270	6.80180
O	8.22860	-5.75570	4.24590
O	8.38570	-1.70680	1.52410
H	9.28110	-1.69300	-0.89990
H	7.93270	-2.50130	-1.30140
H	10.18760	-3.68690	0.15750
H	8.63810	-4.45390	-0.15230
H	8.63240	-4.79450	2.24370
H	7.09290	-2.89510	3.70590
H	8.77840	-2.68230	4.14220
H	6.76690	-6.09020	6.46950
H	8.48310	-5.87740	6.90560
H	7.22380	-4.90700	7.74060

9. GGMe_Trans_GP_Conf_7

N	9.33800	-4.87170	-0.15870
C	9.07220	-3.45290	0.01280
C	8.60920	-2.90720	1.37370
N	8.46150	-3.80580	2.38260
C	8.03460	-3.39980	3.70210
C	7.97270	-4.61410	4.60600
O	7.57480	-4.27890	5.84190
C	7.47940	-5.35810	6.79750
O	8.24860	-5.74670	4.25830
O	8.38570	-1.70640	1.52370
H	8.52270	-5.46280	-0.04220
H	10.10750	-5.21970	0.40210
H	8.31000	-3.14300	-0.71030
H	9.97330	-2.88700	-0.24720
H	8.65410	-4.78930	2.24330
H	7.04960	-2.91780	3.67280
H	8.72070	-2.66080	4.13430
H	6.75630	-6.10190	6.45590
H	8.45430	-5.83220	6.92990
H	7.14670	-4.89160	7.72360

10. GGMe_Trans_GP_Conf_8

N	9.00660	-4.93530	-0.02330
C	9.11520	-3.47380	0.05730
C	8.60520	-2.90230	1.38520
N	8.46370	-3.81740	2.38100
C	7.94100	-3.47280	3.67860
C	6.48590	-3.84660	3.94890
O	5.83240	-4.28960	2.85890
C	4.44100	-4.61540	3.05750
O	5.97960	-3.74200	5.04710
O	8.38750	-1.69970	1.51370
H	8.10610	-5.22170	-0.39640
H	9.72540	-5.33280	-0.61860
H	8.58800	-2.93210	-0.73780
H	10.17090	-3.19030	-0.01450
H	8.62430	-4.78290	2.11480
H	8.01440	-2.38630	3.79170
H	8.53700	-3.92790	4.47620
H	4.33890	-5.40730	3.80310
H	3.89090	-3.73290	3.39150
H	4.08040	-4.94960	2.08520

11. GGMe_Trans_GP_Conf_9

N	9.55620	-4.85160	0.13030
C	9.02250	-3.48780	0.03110
C	8.60530	-2.90240	1.38490
N	8.46370	-3.81720	2.38110
C	8.13890	-3.44100	3.73340
C	9.29640	-3.40470	4.72820
O	10.50460	-3.55070	4.15340
C	11.63280	-3.47720	5.04960
O	9.12690	-3.25020	5.92010
O	8.38750	-1.69990	1.51390
H	9.38190	-5.38500	-0.71470
H	10.55970	-4.84780	0.28910
H	8.11990	-3.50290	-0.58950
H	9.70720	-2.76190	-0.42480
H	8.73780	-4.76530	2.14740
H	7.38020	-4.10780	4.15530
H	7.71340	-2.43250	3.70770
H	11.65810	-2.50400	5.54480
H	11.56990	-4.26410	5.80480
H	12.51170	-3.61300	4.42020

12. GGMe_Trans_GP_Conf_10

N	9.50140	-4.87620	0.12170
C	9.05840	-3.47960	0.03950
C	8.60530	-2.90220	1.38480
N	8.46370	-3.81750	2.38130
C	7.90630	-3.47380	3.66520
C	6.43350	-3.81460	3.88020
O	5.81990	-4.26100	2.76960
C	4.41660	-4.56450	2.91050
O	5.88500	-3.68760	4.95560
O	8.38750	-1.69980	1.51380
H	9.31530	-5.37990	-0.73870
H	10.49790	-4.94320	0.30700
H	8.18550	-3.42080	-0.61960
H	9.80600	-2.78670	-0.36680
H	8.59030	-4.78520	2.10470
H	8.00280	-2.39120	3.79460
H	8.46360	-3.95390	4.47600
H	4.27000	-5.34030	3.66550
H	3.86470	-3.66830	3.20280
H	4.09650	-4.91250	1.92910

13. GGMe_Trans_GP_Conf_11

N	9.06040	-4.94290	-0.00200
C	9.08030	-3.47630	0.04580
C	8.60530	-2.90220	1.38490
N	8.46370	-3.81750	2.38130
C	8.16960	-3.43450	3.73930
C	9.35420	-3.37860	4.70110
O	10.54310	-3.55180	4.09650
C	11.69860	-3.47320	4.95680
O	9.21830	-3.19320	5.89300
O	8.38750	-1.69970	1.51380
H	8.17200	-5.29490	-0.34620
H	9.78930	-5.30850	-0.60520
H	8.48790	-2.98600	-0.73710
H	10.11190	-3.12950	-0.07820
H	8.76690	-4.75850	2.15400
H	7.43120	-4.10810	4.18580
H	7.73110	-2.43180	3.71800
H	11.75500	-2.48700	5.42280
H	11.64470	-4.23750	5.73550
H	12.55540	-3.64240	4.30560

14. GGMe_Trans_GP_Conf_12

N	9.51000	-2.52070	-0.95500
C	9.06780	-3.49190	0.02850
C	8.60860	-2.90180	1.37290
N	8.46160	-3.81300	2.38630
C	7.84410	-3.46330	3.64580
C	6.34920	-3.74850	3.77440
O	5.79840	-4.22600	2.64320
C	4.37830	-4.48040	2.69760
O	5.73640	-3.56170	4.80430
O	8.38630	-1.70460	1.52070
H	10.34600	-2.04520	-0.62400
H	8.80290	-1.79580	-1.05530
H	9.86870	-4.22120	0.20190
H	8.22010	-4.05620	-0.38450
H	8.55080	-4.79320	2.15740
H	7.97680	-2.38850	3.79720
H	8.34090	-3.97600	4.47530
H	4.11390	-4.85470	1.70930
H	4.15540	-5.22230	3.46770
H	3.83930	-3.55670	2.91880

15. GGMe_Trans_GP_Conf_13

N	8.95190	-2.60610	-1.11130
C	9.08360	-3.48910	0.03300
C	8.60860	-2.90180	1.37290
N	8.46160	-3.81310	2.38630
C	8.22660	-3.40540	3.75330
C	9.45800	-3.27780	4.64760
O	10.61500	-3.49580	3.99580
C	11.81500	-3.35270	4.78580
O	9.38110	-3.01030	5.82820
O	8.38630	-1.70450	1.52070
H	7.96990	-2.40980	-1.28920
H	9.37750	-1.70750	-0.89490
H	10.14210	-3.75800	0.15500
H	8.54870	-4.42510	-0.16930
H	8.77370	-4.75970	2.21990
H	7.53960	-4.09740	4.25020
H	7.74580	-2.42360	3.73230
H	11.88690	-2.33640	5.17910
H	11.80850	-4.06210	5.61640
H	12.63720	-3.56170	4.10250

16. GGMe_Trans_GP_Conf_14

N	8.90240	-2.62740	-1.11810
C	9.11110	-3.48350	0.03620
C	8.60950	-2.90600	1.37200
N	8.46130	-3.80630	2.38380
C	8.08080	-3.38160	3.71880
C	7.98750	-4.51380	4.72280
O	8.28990	-5.72080	4.19460
C	8.22160	-6.84360	5.10200
O	7.67400	-4.34540	5.88050
O	8.38570	-1.70710	1.52410
H	9.23970	-1.69090	-0.90590
H	7.90760	-2.52790	-1.30460
H	10.18770	-3.67200	0.14750
H	8.64430	-4.45870	-0.14770
H	8.65180	-4.78700	2.23520
H	7.10860	-2.87520	3.70360
H	8.79440	-2.64890	4.11470
H	8.92650	-6.70450	5.92410
H	7.21060	-6.94090	5.50260
H	8.48840	-7.71430	4.50450

17. GGMe_Trans_GP_Conf_15

N	9.56390	-2.52810	-0.93270
C	9.03940	-3.49450	0.01600
C	8.60950	-2.90600	1.37190
N	8.46130	-3.80640	2.38390
C	7.97290	-3.39780	3.68830
C	7.84680	-4.53470	4.68320
O	8.20370	-5.73350	4.17080
C	8.10470	-6.86070	5.07010
O	7.46290	-4.37650	5.82110
O	8.38570	-1.70700	1.52410
H	8.92570	-1.73750	-0.99270
H	10.44470	-2.14840	-0.59450
H	9.78070	-4.28760	0.17140
H	8.15600	-3.97830	-0.42290
H	8.65050	-4.78730	2.23480
H	6.98820	-2.92190	3.60620
H	8.63370	-2.64440	4.13260
H	8.74820	-6.70530	5.93830
H	7.07180	-6.98630	5.40120
H	8.43460	-7.72200	4.49080

18. GGMe_Trans_GP_Conf_16

N	9.36840	-4.85740	-0.15610
C	9.04340	-3.45080	0.00600
C	8.60810	-2.90270	1.37520
N	8.46200	-3.81300	2.38490
C	8.17330	-3.40860	3.74080
C	9.35680	-3.36980	4.70390
O	10.53420	-3.65730	4.11730
C	11.69090	-3.59970	4.98010
O	9.23020	-3.11040	5.88200
O	8.38640	-1.70380	1.51980
H	8.58820	-5.49020	-0.02560
H	10.18020	-5.16560	0.36580
H	8.24260	-3.18730	-0.69360
H	9.90780	-2.84850	-0.29290
H	8.77610	-4.75710	2.21410
H	7.41670	-4.05950	4.19120
H	7.75790	-2.39730	3.70370
H	11.80460	-2.59330	5.38860
H	11.58750	-4.31320	5.80060
H	12.53800	-3.85680	4.34530

19. GGMe_Trans_GP_Conf_17

N	9.30790	-4.86630	-0.17330
C	9.10100	-3.44170	0.02210
C	8.60810	-2.90270	1.37520
N	8.46200	-3.81290	2.38490
C	7.89490	-3.44950	3.66240
C	6.42860	-3.81200	3.88150
O	5.84600	-4.36290	2.79960
C	4.44740	-4.69140	2.94450
O	5.86040	-3.62160	4.93610
O	8.38640	-1.70380	1.51980
H	10.05200	-5.26730	0.38510
H	8.46580	-5.42670	-0.11690
H	8.38140	-3.08110	-0.72040
H	10.03660	-2.91320	-0.19120
H	8.55240	-4.79090	2.15140
H	7.97420	-2.36300	3.76260
H	8.46110	-3.89870	4.48490
H	4.30920	-5.41310	3.75270
H	3.87060	-3.79000	3.16270
H	4.14990	-5.11780	1.98720

20. GGMe_Trans_GP_Conf_18

N	9.33050	-4.87280	-0.16000
C	9.07420	-3.45220	0.01290
C	8.60920	-2.90640	1.37330
N	8.46150	-3.80640	2.38310
C	8.02670	-3.38520	3.70070
C	7.91820	-4.51470	4.70560
O	8.24590	-5.72170	4.19060
C	8.16110	-6.83920	5.10340
O	7.57160	-4.34660	5.85400
O	8.38580	-1.70660	1.52360
H	10.10040	-5.22720	0.39590
H	8.51160	-5.45990	-0.05000
H	8.31790	-3.13560	-0.71330
H	9.98090	-2.89310	-0.24210
H	8.65260	-4.78500	2.22730
H	7.04760	-2.89400	3.64970
H	8.71290	-2.63790	4.11690
H	8.83820	-6.68700	5.94640
H	7.13920	-6.94450	5.47330
H	8.45550	-7.71130	4.52110

21. GGMe_Cis_GP_Conf_1

N	9.22120	-2.47850	-1.04410
C	9.07670	-3.46560	0.01050
C	8.61090	-2.90550	1.36680
N	8.46040	-3.80440	2.38600
C	8.69350	-5.23040	2.32950
C	8.40110	-5.84570	3.68860
O	8.60550	-7.17150	3.66370
C	8.36140	-7.87570	4.90250
O	8.03380	-5.22330	4.66300
O	8.38520	-1.70950	1.52710
H	9.87360	-1.75660	-0.74660
H	8.33600	-1.99590	-1.18130
H	10.03630	-3.98100	0.15040
H	8.36710	-4.23670	-0.31780
H	8.15430	-3.43210	3.27960
H	9.73140	-5.47840	2.06900
H	8.05370	-5.73360	1.59190
H	8.57720	-8.92060	4.68500
H	9.02060	-7.49740	5.68680
H	7.32090	-7.74890	5.20910

22. GGMe_Cis_GP_Conf_2

N	9.26890	-2.44520	-1.02850
C	9.12780	-3.44520	0.01500
C	8.61260	-2.90400	1.35990
N	8.45920	-3.80350	2.38970
C	8.50480	-5.24210	2.29750
C	7.22680	-5.88190	1.74510
O	7.30530	-7.22360	1.83890
C	6.17530	-7.96480	1.32870
O	6.28490	-5.28110	1.27880
O	8.38470	-1.71190	1.53030
H	9.82730	-1.66820	-0.68220
H	8.35780	-2.04650	-1.24260
H	10.10140	-3.92600	0.18160
H	8.44820	-4.22930	-0.33730
H	8.01840	-3.39970	3.20720
H	8.69640	-5.66290	3.28930
H	9.34090	-5.56780	1.67040
H	6.03690	-7.75790	0.26520
H	6.42180	-9.01340	1.48980
H	5.26820	-7.69120	1.87200

23. GGMe_Cis_GP_Conf_3

N	9.17020	-2.46140	-1.05640
C	9.02390	-3.46150	-0.01380
C	8.61260	-2.90400	1.36000
N	8.45920	-3.80350	2.38960
C	8.86370	-5.18780	2.39870
C	10.36330	-5.40800	2.62400
O	10.61800	-6.72160	2.78040
C	12.00330	-7.08310	2.97370
O	11.20570	-4.53870	2.64600
O	8.38470	-1.71190	1.53030
H	9.91960	-1.81950	-0.80900
H	8.32980	-1.88920	-1.09950
H	9.97080	-4.00320	0.09060
H	8.27370	-4.19920	-0.32970
H	8.29000	-3.35880	3.28370
H	8.59030	-5.68170	1.46060
H	8.31780	-5.71960	3.18390
H	12.00630	-8.16710	3.07920
H	12.59780	-6.77570	2.11060
H	12.39620	-6.60430	3.87330

24. GGMe_Cis_GP_Conf_4

N	10.46240	-3.95120	0.11220
C	9.08280	-3.44630	0.01410
C	8.61060	-2.90710	1.36880
N	8.46070	-3.80390	2.38460
C	8.70790	-5.23030	2.33650
C	8.69970	-5.79260	3.74470
O	8.95790	-7.11150	3.73440
C	8.96470	-7.76590	5.02160
O	8.47880	-5.14670	4.74880
O	8.38520	-1.70850	1.52650
H	11.10170	-3.18680	0.31790
H	10.75690	-4.35490	-0.77300
H	8.43940	-4.27810	-0.29850
H	8.94790	-2.62510	-0.69970
H	8.19550	-3.41880	3.28530
H	9.67310	-5.44310	1.86350
H	7.93840	-5.76950	1.76450
H	9.18950	-8.81060	4.81120
H	9.73000	-7.32620	5.66490
H	7.98810	-7.66780	5.50090

25. GGMe_Cis_GP_Conf_5

N	8.02980	-4.32170	-0.57060
C	9.06430	-3.44900	0.00880
C	8.61060	-2.90700	1.36880
N	8.46070	-3.80390	2.38460
C	8.67560	-5.23520	2.32760
C	8.11130	-5.88170	3.57780
O	8.26570	-7.21620	3.53730
C	7.77660	-7.94560	4.68340
O	7.59910	-5.28010	4.49980
O	8.38520	-1.70850	1.52660
H	8.35230	-4.72130	-1.44780
H	7.19270	-3.78240	-0.77940
H	9.31070	-2.56960	-0.59800
H	9.97800	-4.04350	0.13300
H	8.11180	-3.43120	3.26180
H	9.74290	-5.49670	2.27750
H	8.19330	-5.66660	1.44350
H	6.70360	-7.78200	4.80560
H	7.98640	-8.99240	4.46820
H	8.29770	-7.62300	5.58760

26. GGMe_Cis_GP_Conf_6

N	9.16320	-2.46380	-1.05800
C	9.04460	-3.45930	-0.00820
C	8.61230	-2.90460	1.36130
N	8.45940	-3.80340	2.38880
C	8.86900	-5.18910	2.40080
C	10.34240	-5.49110	2.69740
O	11.07610	-4.38850	2.91530
C	12.47540	-4.60700	3.20250
O	10.77640	-6.62370	2.72920
O	8.38480	-1.71140	1.52980
H	9.83150	-1.75000	-0.77740
H	8.27810	-1.97400	-1.16630
H	10.00770	-3.97240	0.10390
H	8.32400	-4.22470	-0.32460
H	8.26360	-3.36280	3.27950
H	8.63680	-5.67320	1.44820
H	8.28710	-5.72870	3.15480
H	12.89680	-3.61360	3.34950
H	12.58430	-5.21400	4.10390
H	12.95710	-5.11480	2.36410

27. GGMe_Cis_GP_Conf_7

N	9.27680	-2.44540	-1.02560
C	9.11050	-3.44880	0.01030
C	8.61230	-2.90460	1.36140
N	8.45940	-3.80350	2.38880
C	8.49670	-5.24500	2.29580
C	7.22340	-5.95870	1.82770
O	6.21460	-5.11730	1.55240
C	4.98440	-5.73010	1.10610
O	7.15890	-7.16620	1.72720
O	8.38480	-1.71130	1.52970
H	9.92280	-1.72750	-0.70570
H	8.39420	-1.96300	-1.17810
H	10.06910	-3.96070	0.16590
H	8.40920	-4.21360	-0.34580
H	8.04390	-3.39610	3.21770
H	8.73910	-5.66230	3.27830
H	9.30040	-5.57230	1.63050
H	5.15520	-6.28920	0.18360
H	4.60080	-6.40630	1.87310
H	4.29640	-4.90280	0.93770

28. GGMe_Cis_GP_Conf_8

N	9.21990	-2.47690	-1.04490
C	9.07730	-3.46460	0.00900
C	8.61140	-2.90580	1.36520
N	8.46010	-3.80370	2.38660
C	8.69380	-5.23400	2.32450
C	8.43950	-5.96040	3.63720
O	8.03730	-5.14470	4.62820
C	7.77760	-5.77310	5.90450
O	8.59010	-7.15680	3.75730
O	8.38500	-1.70990	1.52810
H	9.87160	-1.75390	-0.74850
H	8.33390	-1.99650	-1.18420
H	10.03760	-3.97880	0.14850
H	8.36930	-4.23700	-0.31930
H	8.15350	-3.41550	3.26990
H	9.72940	-5.47070	2.04720
H	8.05140	-5.72490	1.58160
H	7.46860	-4.96450	6.56510
H	6.98530	-6.51700	5.80030
H	8.68430	-6.25540	6.27480

29. GGMe_Cis_GP_Conf_9

N	10.36250	-4.16690	0.10940
C	9.09440	-3.42680	0.00420
C	8.61250	-2.90600	1.36120
N	8.45940	-3.80200	2.38820
C	8.50230	-5.24450	2.31270
C	7.21130	-5.88130	1.80410
O	7.18390	-7.19470	2.11250
C	6.04480	-7.93720	1.62950
O	6.34150	-5.31210	1.18020
O	8.38460	-1.71140	1.53050
H	11.11510	-3.54450	0.39430
H	10.62180	-4.55080	-0.79540
H	8.33080	-4.10440	-0.39480
H	9.13590	-2.54530	-0.64620
H	8.04880	-3.38270	3.21360
H	8.73500	-5.65510	3.29910
H	9.31670	-5.54150	1.64170
H	6.19760	-8.95860	1.97620
H	5.12100	-7.52280	2.03940
H	6.00340	-7.90120	0.53840

30. GGMe_Cis_GP_Conf_10

N	8.16590	-4.49690	-0.50590
C	9.05310	-3.43320	-0.00740
C	8.61260	-2.90610	1.36110
N	8.45940	-3.80190	2.38820
C	8.85650	-5.19120	2.41240
C	10.34350	-5.41110	2.67980
O	10.56640	-6.68380	3.06850
C	11.94510	-7.04890	3.28830
O	11.21690	-4.58290	2.53370
O	8.38460	-1.71140	1.53060
H	8.52180	-4.87000	-1.38180
H	7.23810	-4.12600	-0.69610
H	9.10970	-2.54970	-0.65380
H	10.06410	-3.84470	0.09140
H	8.25680	-3.35110	3.27210
H	8.61330	-5.64740	1.44560
H	8.27730	-5.72340	3.17200
H	12.38210	-6.42410	4.07050
H	11.92160	-8.09370	3.59570
H	12.52050	-6.92910	2.36740

31. GGMe_Cis_GP_Conf_11

N	8.22190	-4.45240	-0.54340
C	9.11400	-3.42400	0.01070
C	8.61230	-2.90610	1.36190
N	8.45950	-3.80210	2.38780
C	8.55060	-5.24210	2.33360
C	7.22010	-5.92970	2.03190
O	7.41530	-7.25010	1.84320
C	6.23380	-8.03230	1.57660
O	6.13630	-5.38960	2.01040
O	8.38460	-1.71130	1.53020
H	8.57960	-4.78570	-1.43460
H	7.29690	-4.06530	-0.71670
H	9.23070	-2.53120	-0.61510
H	10.10830	-3.87030	0.14470
H	8.01060	-3.39440	3.19910
H	8.90710	-5.61550	3.30140
H	9.27580	-5.55870	1.58460
H	5.75290	-7.68720	0.65840
H	6.58410	-9.05800	1.46630
H	5.52780	-7.95120	2.40650

32. GGMe_Cis_GP_Conf_12

N	10.32360	-4.13880	0.04750
C	9.03420	-3.43590	-0.01190
C	8.61240	-2.90610	1.36180
N	8.45950	-3.80200	2.38780
C	8.80500	-5.20390	2.40580
C	10.23350	-5.47820	2.87300
O	10.52820	-6.78400	2.71390
C	11.84240	-7.19270	3.14350
O	10.98440	-4.66320	3.36170
O	8.38460	-1.71130	1.53020
H	11.06210	-3.50430	0.34280
H	10.57730	-4.48850	-0.87250
H	8.27540	-4.14360	-0.37130
H	9.01660	-2.56300	-0.67530
H	8.29840	-3.35080	3.28010
H	8.67700	-5.64970	1.41980
H	8.12480	-5.73160	3.08540
H	11.89020	-8.26410	2.95140
H	12.60740	-6.66300	2.57100
H	11.97790	-6.98340	4.20720

33. GGMe_Cis_GP_Conf_13

N	8.84540	-2.45710	-1.03070
C	9.07090	-3.44890	0.00820
C	8.61230	-2.90520	1.36170
N	8.45950	-3.80280	2.38830
C	8.90340	-5.17770	2.41330
C	10.38330	-5.43660	2.71450
O	11.04430	-4.33300	3.09860
C	12.44120	-4.51330	3.42060
O	10.87980	-6.54030	2.62830
O	8.38470	-1.71140	1.52990
H	9.56600	-2.48320	-1.74260
H	8.81550	-1.52960	-0.61240
H	10.12970	-3.73840	0.12940
H	8.52020	-4.37060	-0.22300
H	8.27160	-3.35420	3.27630
H	8.68240	-5.67710	1.46680
H	8.33400	-5.72030	3.17540
H	12.80040	-3.52530	3.70490
H	12.54930	-5.22020	4.24600
H	12.98310	-4.88880	2.54980

34. GGMe_Cis_GP_Conf_14

N	9.52100	-2.35560	-0.84090
C	9.07690	-3.44800	0.00980
C	8.61230	-2.90520	1.36160
N	8.45950	-3.80270	2.38830
C	8.46330	-5.24420	2.29080
C	7.17850	-5.92350	1.80530
O	6.14720	-5.07360	1.67890
C	4.89840	-5.65540	1.24320
O	7.11890	-7.11490	1.58290
O	8.38470	-1.71150	1.53000
H	9.07880	-1.49010	-0.53890
H	9.30400	-2.52270	-1.81660
H	9.89490	-4.16460	0.16300
H	8.22960	-4.02250	-0.40430
H	8.03770	-3.38900	3.21050
H	8.68060	-5.66580	3.27790
H	9.26850	-5.59000	1.63780
H	5.01990	-6.11510	0.25990
H	4.56610	-6.41210	1.95720
H	4.19460	-4.82550	1.19970

35. GGMe_Cis_GP_Conf_15

N	8.17760	-4.49310	-0.51040
C	9.06170	-3.43250	-0.00450
C	8.61230	-2.90660	1.36240
N	8.45960	-3.80200	2.38750
C	8.85430	-5.19470	2.41670
C	10.29130	-5.49750	2.83540
O	11.11850	-4.44550	2.69100
C	12.49970	-4.67700	3.04080
O	10.64620	-6.59190	3.22370
O	8.38460	-1.71080	1.53000
H	8.52800	-4.85660	-1.39250
H	7.24510	-4.12720	-0.68730
H	9.12740	-2.54750	-0.64830
H	10.07110	-3.84860	0.09870
H	8.22520	-3.35610	3.26610
H	8.69480	-5.62570	1.42210
H	8.20640	-5.74520	3.10430
H	13.00270	-3.72540	2.87370
H	12.57840	-4.97910	4.08740
H	12.92460	-5.45930	2.40750

36. GGMe_Cis_GP_Conf_16

N	10.35680	-4.16440	0.10220
C	9.08730	-3.42890	0.00280
C	8.61230	-2.90660	1.36250
N	8.45960	-3.80200	2.38740
C	8.50350	-5.24750	2.31810
C	7.20010	-5.96280	1.96910
O	6.31110	-5.16940	1.34290
C	5.06890	-5.79560	0.95790
O	7.01160	-7.13870	2.20590
O	8.38460	-1.71080	1.53000
H	11.10690	-3.54470	0.39860
H	10.62090	-4.54050	-0.80430
H	8.32560	-4.11230	-0.39170
H	9.11950	-2.54900	-0.65040
H	8.08030	-3.37820	3.22550
H	8.83300	-5.65110	3.27940
H	9.25780	-5.54060	1.57940
H	4.48330	-5.00780	0.48560
H	5.25790	-6.61350	0.25870
H	4.55450	-6.18660	1.83850

37. GGMe_Cis_GP_Conf_17

N	8.12020	-4.38160	-0.55480
C	9.09400	-3.43750	0.01020
C	8.61210	-2.90630	1.36290
N	8.45970	-3.80260	2.38740
C	8.54530	-5.24530	2.32850
C	7.26250	-6.00590	1.99380
O	6.15720	-5.24920	2.10650
C	4.91020	-5.91820	1.83120
O	7.25760	-7.18860	1.72350
O	8.38470	-1.71050	1.52950
H	8.49350	-4.83030	-1.38650
H	7.27190	-3.89300	-0.83030
H	9.28680	-2.55100	-0.60560
H	10.04580	-3.96670	0.14300
H	8.04200	-3.39100	3.21290
H	8.88390	-5.61770	3.30280
H	9.29060	-5.56180	1.59920
H	4.13850	-5.16270	1.97470
H	4.90220	-6.29120	0.80440
H	4.76740	-6.75520	2.51870

38. GGMe_Cis_GP_Conf_18

N	10.39530	-4.03850	0.08430
C	9.05450	-3.44370	-0.00080
C	8.61210	-2.90630	1.36300
N	8.45970	-3.80260	2.38740
C	8.81530	-5.20450	2.40390
C	10.24150	-5.55630	2.82650
O	10.87880	-4.53700	3.42800
C	12.22070	-4.81500	3.87580
O	10.70760	-6.66760	2.68640
O	8.38470	-1.71050	1.52950
H	11.09390	-3.31650	0.24200
H	10.63740	-4.50820	-0.78360
H	8.35550	-4.22190	-0.33130
H	8.96830	-2.59930	-0.69510
H	8.26660	-3.35720	3.27590
H	8.66390	-5.65650	1.42390
H	8.14610	-5.72910	3.09650
H	12.56980	-3.89100	4.33550
H	12.21860	-5.63290	4.60010
H	12.85130	-5.08860	3.02660

39. GGMe_Cis_GP_Conf_19

N	8.04250	-4.32430	-0.57630
C	9.06880	-3.44520	0.00680
C	8.61110	-2.90730	1.36690
N	8.46040	-3.80310	2.38530
C	8.68950	-5.23620	2.33060
C	7.99470	-6.01820	3.43090
O	7.33680	-5.23550	4.30920
C	6.66330	-5.92020	5.38790
O	8.05090	-7.22690	3.51100
O	8.38500	-1.70900	1.52770
H	8.36900	-4.72070	-1.45340
H	7.19990	-3.79330	-0.78360
H	9.31060	-2.56310	-0.59780
H	9.98630	-4.03330	0.13240
H	8.12790	-3.40850	3.25630
H	9.75680	-5.48890	2.41370
H	8.33020	-5.63140	1.37460
H	7.38300	-6.48970	5.97970
H	6.20340	-5.13400	5.98500
H	5.90640	-6.59740	4.98690

40. GGMe_Cis_GP_Conf_20

N	10.45220	-3.96460	0.10140
C	9.07910	-3.44390	0.00960
C	8.61120	-2.90740	1.36680
N	8.46030	-3.80300	2.38530
C	8.69180	-5.23590	2.33200
C	8.91020	-5.88010	3.68950
O	8.78070	-5.01800	4.71720
C	8.96590	-5.57310	6.03800
O	9.15630	-7.06010	3.82230
O	8.38500	-1.70910	1.52780
H	11.10200	-3.21140	0.31390
H	10.74140	-4.36730	-0.78590
H	8.42540	-4.26640	-0.30630
H	8.95110	-2.61720	-0.69900
H	8.17950	-3.40040	3.27070
H	9.58000	-5.44440	1.72660
H	7.84730	-5.77530	1.87850
H	8.81920	-4.73970	6.72360
H	8.23360	-6.36250	6.22020
H	9.97330	-5.98330	6.13360

41. GGMe_Trans_WP_Conf_1

N	9.31850	-4.88390	-0.13810
C	9.07150	-3.45000	0.01880
C	8.60910	-2.91630	1.37910
N	8.46260	-3.80680	2.37930
C	7.92850	-3.45350	3.67550
C	6.40000	-3.42790	3.68960
O	5.94600	-3.10850	4.90760
C	4.50260	-3.04360	5.08750
O	5.68070	-3.66540	2.73400
O	8.38480	-1.69640	1.52160
H	8.48300	-5.44430	0.03820
H	10.06360	-5.22010	0.47410
H	8.30520	-3.12980	-0.69920
H	9.97740	-2.88810	-0.24140
H	8.63810	-4.78820	2.19110
H	8.29040	-2.46500	3.98120
H	8.27240	-4.17860	4.42110
H	4.35840	-2.79270	6.13810
H	4.08290	-2.26840	4.44280
H	4.05530	-4.01250	4.85550

42. GGMe_Trans_WP_Conf_2

N	9.30370	-4.88490	-0.14570
C	9.07310	-3.44870	0.01830
C	8.60930	-2.91630	1.37820
N	8.46250	-3.80630	2.37960
C	8.12640	-3.41370	3.73000
C	9.33390	-2.88580	4.50480
O	8.96390	-2.46810	5.72150
C	10.00380	-1.94900	6.59740
O	10.48030	-2.85030	4.09090
O	8.38470	-1.69690	1.52210
H	8.45930	-5.43460	0.02130
H	10.03910	-5.23400	0.47110
H	8.33110	-3.10820	-0.71460
H	9.99600	-2.90160	-0.21440
H	8.68030	-4.78220	2.20860
H	7.72350	-4.27930	4.26720
H	7.35340	-2.63660	3.72580
H	9.49320	-1.69960	7.52750
H	10.76420	-2.71420	6.76720
H	10.45370	-1.05870	6.15260

43. GGMe_Trans_WP_Conf_3

N	9.59100	-4.81340	0.01960
C	9.04190	-3.44830	0.01110
C	8.60950	-2.91680	1.37760
N	8.46230	-3.80540	2.37950
C	8.10470	-3.40260	3.72470
C	9.28820	-2.82800	4.50700
O	8.86710	-2.20210	5.61420
C	9.88080	-1.62170	6.48480
O	10.46040	-2.92980	4.18710
O	8.38460	-1.69720	1.52280
H	10.56580	-4.79730	0.32790
H	9.61250	-5.17410	-0.93690
H	8.14420	-3.42590	-0.62010
H	9.72820	-2.69460	-0.39870
H	8.67020	-4.78010	2.18400
H	7.72730	-4.27260	4.27490
H	7.30730	-2.65220	3.70380
H	9.32400	-1.11340	7.27220
H	10.50670	-2.41250	6.90420
H	10.49220	-0.91140	5.92460

44. GGMe_Trans_WP_Conf_4

N	9.03870	-4.90050	-0.13440
C	9.09840	-3.43950	0.02680
C	8.60960	-2.91680	1.37750
N	8.46230	-3.80540	2.37950
C	7.95770	-3.42380	3.68330
C	6.43570	-3.26420	3.70760
O	6.04190	-2.62820	4.81900
C	4.61140	-2.42410	5.00600
O	5.67130	-3.66860	2.84760
O	8.38460	-1.69730	1.52280
H	9.60790	-5.17420	-0.93830
H	8.08510	-5.19130	-0.36090
H	8.52990	-2.88350	-0.73150
H	10.14150	-3.11050	-0.06540
H	8.65870	-4.78180	2.18130
H	8.40970	-2.48160	4.01110
H	8.22730	-4.19400	4.41560
H	4.11060	-3.38860	5.11590
H	4.52400	-1.83860	5.92140
H	4.19800	-1.87680	4.15650

45. GGMe_Trans_WP_Conf_5

N	9.07900	-4.90410	-0.11890
C	9.10200	-3.44060	0.02930
C	8.60920	-2.91680	1.37880
N	8.46260	-3.80620	2.37920
C	8.05240	-3.42280	3.71590
C	6.54840	-3.29620	3.96150
O	5.78640	-3.79130	2.98910
C	4.34260	-3.72690	3.17070
O	6.10860	-2.79830	4.99060
O	8.38470	-1.69640	1.52190
H	9.67940	-5.17470	-0.90080
H	8.13970	-5.22020	-0.36940
H	8.51970	-2.90570	-0.73340
H	10.13680	-3.08690	-0.06670
H	8.68080	-4.77820	2.17930
H	8.49130	-2.45570	3.98360
H	8.42610	-4.16360	4.43280
H	4.01890	-2.68440	3.21310
H	3.92490	-4.22560	2.29610
H	4.05810	-4.24980	4.08650

46. GGMe_Trans_WP_Conf_6

N	9.02480	-4.92420	-0.09640
C	9.09970	-3.46170	0.03700
C	8.60890	-2.91880	1.38090
N	8.46290	-3.80420	2.37700
C	8.02560	-3.43440	3.71120
C	8.07170	-4.64210	4.62890
O	7.70130	-4.31700	5.86870
C	7.69070	-5.37200	6.87450
O	8.40080	-5.76590	4.27890
O	8.38470	-1.69640	1.52190
H	9.63970	-5.23240	-0.85170
H	8.08240	-5.21010	-0.37030
H	8.54550	-2.91230	-0.73590
H	10.14810	-3.14850	-0.04860
H	8.67790	-4.77740	2.18070
H	6.99740	-3.04510	3.70290
H	8.66470	-2.64800	4.13470
H	7.01430	-6.17250	6.56810
H	8.70190	-5.75990	7.01520
H	7.33210	-4.89050	7.78430

47. GGMe_Trans_WP_Conf_7

N	9.38190	-4.87190	-0.12420
C	9.06760	-3.44960	0.01680
C	8.60910	-2.91650	1.37900
N	8.46260	-3.80670	2.37920
C	7.98570	-3.44600	3.69760
C	6.46740	-3.38500	3.86370
O	5.78440	-3.71260	2.77010
C	4.33090	-3.67840	2.84790
O	5.95090	-3.06500	4.92740
O	8.38480	-1.69630	1.52160
H	8.56940	-5.46850	0.03940
H	10.13000	-5.17110	0.50370
H	8.27350	-3.18010	-0.69190
H	9.93880	-2.84730	-0.27030
H	8.64510	-4.78700	2.19230
H	8.37550	-2.46300	3.98540
H	8.36000	-4.17500	4.42490
H	3.99500	-2.67150	3.10590
H	3.98710	-3.95700	1.85180
H	3.98260	-4.39760	3.59270

48. GGMe_Trans_WP_Conf_8

N	9.27240	-4.88820	-0.15360
C	9.07600	-3.44820	0.01930
C	8.60910	-2.91650	1.37900
N	8.46260	-3.80670	2.37930
C	8.08080	-3.43140	3.72420
C	9.21610	-2.96100	4.63280
O	10.41890	-2.99200	4.06510
C	11.55380	-2.55980	4.86800
O	9.00780	-2.59820	5.78420
O	8.38480	-1.69630	1.52160
H	8.41870	-5.42070	0.02250
H	10.00900	-5.25610	0.45040
H	8.35020	-3.08180	-0.71760
H	10.01460	-2.92280	-0.20120
H	8.67960	-4.78190	2.20260
H	7.61100	-4.29100	4.21480
H	7.34160	-2.62270	3.69620
H	11.66330	-3.21260	5.73700
H	12.41720	-2.64700	4.20840
H	11.41280	-1.52440	5.18620

49. GGMe_Trans_WP_Conf_9

N	9.57370	-4.82070	0.01510
C	9.04050	-3.44990	0.01150
C	8.60940	-2.91690	1.37840
N	8.46250	-3.80560	2.37920
C	8.02300	-3.42210	3.70740
C	9.09580	-2.86900	4.64690
O	10.34460	-3.05730	4.22780
C	11.42070	-2.57520	5.08420
O	8.80200	-2.32460	5.70420
O	8.38470	-1.69690	1.52240
H	10.55260	-4.81730	0.30970
H	9.57540	-5.18570	-0.93980
H	8.14180	-3.41640	-0.61830
H	9.73370	-2.70270	-0.39860
H	8.65460	-4.78210	2.17580
H	7.58590	-4.29580	4.20510
H	7.24350	-2.65560	3.64230
H	11.34550	-3.03410	6.07230
H	12.33860	-2.88360	4.58390
H	11.37100	-1.48690	5.16510

50. GGMe_Trans_WP_Conf_10

N	8.86310	-4.87230	-0.20850
C	9.10430	-3.43980	0.02640
C	8.61050	-2.91810	1.37490
N	8.46180	-3.80230	2.37970
C	8.02070	-3.38880	3.69820
C	9.07610	-2.58300	4.45960
O	8.50270	-1.79330	5.37690
C	9.37610	-0.98960	6.22020
O	10.28170	-2.66050	4.28630
O	8.38420	-1.69900	1.52530
H	9.39160	-5.16780	-1.03290
H	7.87970	-5.02510	-0.44490
H	8.66310	-2.77990	-0.73170
H	10.18700	-3.25640	0.00950
H	8.70100	-4.77340	2.20610
H	7.79400	-4.28250	4.29300
H	7.10590	-2.79060	3.63130
H	8.70500	-0.38480	6.83020
H	9.98780	-1.63970	6.84990
H	10.01250	-0.35360	5.60140

51. GGMe_Trans_WP_Conf_11

N	9.77080	-4.72590	0.04260
C	9.03800	-3.45080	0.00760
C	8.61060	-2.91790	1.37450
N	8.46170	-3.80210	2.37980
C	8.03430	-3.38490	3.70190
C	6.56840	-2.94610	3.74840
O	6.35850	-2.08980	4.75640
C	4.99960	-1.60860	4.96610
O	5.69290	-3.33780	2.99380
O	8.38420	-1.69940	1.52550
H	10.73610	-4.56330	0.33910
H	9.83540	-5.10040	-0.90670
H	8.11150	-3.59010	-0.56530
H	9.58540	-2.63200	-0.47720
H	8.62170	-4.78520	2.18470
H	8.65680	-2.56230	4.06970
H	8.14970	-4.22840	4.39390
H	5.07690	-0.88550	5.77820
H	4.62860	-1.12920	4.05780
H	4.35010	-2.43950	5.25040

52. GGMe_Trans_WP_Conf_12

N	9.31840	-4.90730	-0.10750
C	9.07260	-3.47080	0.02850
C	8.60840	-2.91880	1.38280
N	8.46320	-3.80480	2.37620
C	8.03250	-3.47580	3.72110
C	7.99100	-4.75720	4.53690
O	7.59250	-4.53640	5.78960
C	7.51150	-5.69210	6.67320
O	8.28790	-5.85810	4.09370
O	8.38490	-1.69590	1.52090
H	8.48410	-5.46850	0.07580
H	10.07390	-5.23750	0.49630
H	8.31720	-3.15940	-0.70350
H	9.98640	-2.92150	-0.23060
H	8.66180	-4.78260	2.19700
H	7.03370	-3.01770	3.72310
H	8.71990	-2.76690	4.20340
H	8.49760	-6.15080	6.77250
H	7.16860	-5.29490	7.62790
H	6.79780	-6.41470	6.27200

53. GGMe_Trans_WP_Conf_13

N	9.83820	-2.57500	-0.79790
C	9.05010	-3.49660	0.02610
C	8.61010	-2.91670	1.37560
N	8.46190	-3.80290	2.37960
C	8.02300	-3.40200	3.70550
C	8.10930	-4.57330	4.66330
O	7.81080	-4.19440	5.90690
C	7.85870	-5.20410	6.95590
O	8.41340	-5.71210	4.34070
O	8.38450	-1.69980	1.52460
H	10.71010	-2.34250	-0.31640
H	9.33730	-1.68940	-0.89730
H	9.61530	-4.42270	0.18270
H	8.13440	-3.77700	-0.51230
H	8.67330	-4.78460	2.22380
H	6.98740	-3.03400	3.69680
H	8.64740	-2.58720	4.09320
H	7.11820	-5.98130	6.75700
H	8.86010	-5.63590	7.00900
H	7.61970	-4.66700	7.87370

54. GGMe_Trans_WP_Conf_14

N	9.83870	-4.69360	0.06830
C	9.04210	-3.45670	0.01090
C	8.61040	-2.91780	1.37510
N	8.46180	-3.80240	2.37970
C	8.12950	-3.38710	3.72980
C	6.69320	-2.92140	3.97120
O	5.80250	-3.40550	3.10640
C	4.40950	-3.02530	3.30130
O	6.40210	-2.19980	4.91670
O	8.38420	-1.69920	1.52510
H	10.78330	-4.48110	0.39860
H	9.95640	-5.05800	-0.88010
H	8.11960	-3.65610	-0.55040
H	9.54550	-2.62290	-0.49530
H	8.64890	-4.78140	2.18860
H	8.77590	-2.56250	4.04960
H	8.30850	-4.23050	4.40780
H	4.29720	-1.94680	3.16880
H	3.85680	-3.56720	2.53420
H	4.07620	-3.32040	4.29860

55. GGMe_Trans_WP_Conf_15

N	8.70940	-4.83210	-0.26820
C	9.10980	-3.44650	0.02860
C	8.61080	-2.91790	1.37390
N	8.46160	-3.80150	2.38000
C	7.93240	-3.40820	3.67370
C	8.83150	-2.52390	4.53820
O	10.13630	-2.67610	4.31210
C	11.05020	-1.88610	5.12720
O	8.37240	-1.78120	5.39650
O	8.38410	-1.70000	1.52600
H	9.19630	-5.14280	-1.11230
H	7.71390	-4.85970	-0.50310
H	8.78090	-2.71590	-0.72110
H	10.20620	-3.39610	0.06140
H	8.67060	-4.77840	2.20080
H	7.72390	-4.31540	4.25400
H	6.98950	-2.86280	3.55740
H	10.88850	-2.09940	6.18600
H	12.04800	-2.19780	4.81920
H	10.89970	-0.82250	4.92870

56. GGMe_Trans_WP_Conf_16

N	9.57390	-4.83820	0.05560
C	9.04210	-3.46800	0.01960
C	8.60910	-2.91830	1.38000
N	8.46270	-3.80440	2.37760
C	8.03980	-3.41140	3.71370
C	7.77010	-4.57250	4.65310
O	7.94520	-5.77400	4.10600
C	7.69590	-6.94040	4.94620
O	7.42000	-4.38970	5.81130
O	8.38470	-1.69670	1.52230
H	10.56680	-4.82900	0.29790
H	9.51960	-5.25240	-0.87640
H	8.14430	-3.44680	-0.61120
H	9.73720	-2.72960	-0.40210
H	8.65380	-4.77840	2.16820
H	7.11550	-2.82030	3.66530
H	8.79680	-2.77800	4.19730
H	6.66380	-6.92340	5.30380
H	7.86760	-7.79800	4.29590
H	8.39240	-6.94370	5.78790

57. GGMe_Trans_WP_Conf_17

N	7.99250	-3.23570	-1.02570
C	9.02270	-3.46430	0.00580
C	8.61130	-2.91660	1.37120
N	8.46120	-3.80230	2.38190
C	7.90270	-3.37430	3.65320
C	6.44310	-2.93800	3.49900
O	6.11640	-1.98040	4.37430
C	4.75170	-1.47310	4.32670
O	5.66380	-3.41120	2.68740
O	8.38400	-1.70040	1.52670
H	7.75280	-2.24220	-1.06640
H	7.12870	-3.72420	-0.77800
H	9.94400	-2.94970	-0.29130
H	9.24670	-4.53400	0.06350
H	8.59310	-4.79490	2.20730
H	8.48040	-2.54770	4.07770
H	7.93800	-4.21210	4.35850
H	4.04800	-2.26990	4.57630
H	4.71680	-0.67860	5.07170
H	4.53790	-1.07840	3.33100

58. GGMe_Trans_WP_Conf_18

N	10.48160	-2.99730	-0.28430
C	9.11650	-3.45870	0.03820
C	8.61040	-2.91570	1.37400
N	8.46170	-3.80510	2.38150
C	8.11730	-3.37740	3.72480
C	9.22780	-2.65230	4.48620
O	10.43730	-2.80920	3.95370
C	11.55460	-2.14630	4.60730
O	9.00340	-2.00990	5.50420
O	8.38440	-1.69870	1.52440
H	10.52870	-1.97640	-0.24450
H	11.14580	-3.34190	0.41240
H	9.09570	-4.55320	0.02770
H	8.42920	-3.10700	-0.73960
H	8.70170	-4.78040	2.22640
H	7.83240	-4.25460	4.31660
H	7.25780	-2.69910	3.70550
H	11.64450	-2.49180	5.63950
H	12.43160	-2.43260	4.02690
H	11.41190	-1.06320	4.58000

59. GGMe_Trans_WP_Conf_19

N	7.94340	-3.38910	-0.99100
C	9.02490	-3.47220	0.01120
C	8.61070	-2.91620	1.37310
N	8.46150	-3.80380	2.38150
C	7.94290	-3.39410	3.67450
C	6.47420	-2.96830	3.67820
O	5.77690	-3.44020	2.64690
C	4.37090	-3.07840	2.55900
O	5.99710	-2.28160	4.57240
O	8.38420	-1.69950	1.52530
H	7.59580	-2.42950	-1.05760
H	7.14790	-3.96230	-0.70180
H	9.87880	-2.88060	-0.33750
H	9.35550	-4.51220	0.09730
H	8.61340	-4.79320	2.20530
H	8.04660	-4.22790	4.37820
H	8.51410	-2.54910	4.07310
H	3.83790	-3.42160	3.44840
H	4.27140	-1.99570	2.45020
H	4.00320	-3.58840	1.66870

60. GGMe_Trans_WP_Conf_20

N	10.44710	-2.89050	-0.31350
C	9.12590	-3.44770	0.03520
C	8.61130	-2.91640	1.37130
N	8.46120	-3.80270	2.38200
C	8.17120	-3.33510	3.72680
C	9.34810	-2.54340	4.30410
O	8.94110	-1.60750	5.16890
C	9.97020	-0.78390	5.78990
O	10.51850	-2.74450	4.02180
O	8.38400	-1.70040	1.52660
H	11.14380	-3.16980	0.38120
H	10.41360	-1.86870	-0.28360
H	9.18270	-4.54060	0.04110
H	8.40180	-3.15770	-0.73490
H	8.71870	-4.77580	2.24130
H	7.98720	-4.19900	4.37500
H	7.27690	-2.70520	3.73750
H	10.54240	-0.26350	5.01870
H	9.42890	-0.07290	6.41360
H	10.63150	-1.40710	6.39530

61. GGMe_Trans_WP_Conf_21

N	9.33760	-4.90280	-0.11040
C	9.07170	-3.46950	0.02580
C	8.60870	-2.91840	1.38130
N	8.46290	-3.80440	2.37690
C	8.03560	-3.45210	3.72130
C	7.95720	-4.65680	4.64370
O	8.28400	-5.80380	4.04830
C	8.24280	-7.02710	4.83710
O	7.62330	-4.55970	5.81570
O	8.38480	-1.69660	1.52170
H	8.50990	-5.47990	0.04930
H	10.09150	-5.22660	0.49810
H	8.30610	-3.17070	-0.70090
H	9.97400	-2.90460	-0.23880
H	8.66130	-4.77890	2.19040
H	7.04230	-2.98200	3.70940
H	8.72790	-2.73190	4.17920
H	7.22770	-7.19500	5.20440
H	8.54140	-7.81640	4.14680
H	8.94510	-6.95220	5.67050

62. GGMe_Trans_WP_Conf_22

N	8.81950	-2.64070	-1.12470
C	9.10540	-3.48660	0.03770
C	8.61070	-2.91660	1.37340
N	8.46150	-3.80180	2.38050
C	8.04470	-3.37080	3.70840
C	7.91040	-4.49180	4.71960
O	8.22700	-5.69480	4.24460
C	8.12410	-6.82640	5.15620
O	7.54260	-4.28010	5.86760
O	8.38430	-1.70110	1.52600
H	9.17320	-1.69630	-0.95650
H	7.80840	-2.53410	-1.23330
H	10.19150	-3.62520	0.13060
H	8.67760	-4.48400	-0.11920
H	8.64410	-4.78640	2.21750
H	7.07200	-2.86280	3.66330
H	8.75550	-2.64480	4.12630
H	7.08790	-6.94150	5.48370
H	8.44680	-7.68920	4.57380
H	8.77960	-6.66840	6.01600

63. GGMe_Trans_WP_Conf_23

N	9.82070	-2.56180	-0.80590
C	9.04480	-3.49210	0.02140
C	8.61030	-2.91650	1.37460
N	8.46170	-3.80270	2.38020
C	8.01310	-3.38690	3.70280
C	8.06740	-4.48150	4.75070
O	8.40830	-5.67590	4.27120
C	8.48110	-6.78630	5.21250
O	7.80580	-4.26030	5.92510
O	8.38440	-1.70030	1.52510
H	10.69700	-2.33020	-0.33230
H	9.31520	-1.67720	-0.89250
H	9.61770	-4.41480	0.16890
H	8.12640	-3.77470	-0.51150
H	8.66950	-4.78250	2.21970
H	6.97670	-3.02150	3.67460
H	8.62890	-2.55680	4.07060
H	7.51470	-6.91720	5.70500
H	8.72980	-7.65560	4.60390
H	9.26310	-6.59040	5.95020

64. GGMe_Cis_WP_Conf_1

N	9.33210	-2.41330	-1.00490
C	9.03860	-3.45390	-0.01660
C	8.61400	-2.91820	1.36250
N	8.45960	-3.79580	2.38420
C	8.74100	-5.21930	2.38740
C	10.16610	-5.55710	2.83790
O	10.27130	-6.85640	3.13890
C	11.57460	-7.34940	3.56760
O	11.08820	-4.76140	2.90270
O	8.38290	-1.70540	1.53330
H	8.52750	-1.79010	-1.10170
H	10.09430	-1.82110	-0.66690
H	9.91680	-4.10080	0.08960
H	8.22810	-4.09350	-0.39490
H	8.17830	-3.37980	3.27110
H	8.59420	-5.65770	1.39380
H	8.03610	-5.72250	3.05780
H	11.92190	-6.78030	4.43220
H	11.40870	-8.39300	3.83480
H	12.29090	-7.27020	2.74670

65. GGMe_Cis_WP_Conf_2

N	9.12290	-2.43870	-1.06330
C	9.11750	-3.44140	0.00530
C	8.61410	-2.91840	1.36240
N	8.45960	-3.79540	2.38400
C	8.61370	-5.23800	2.35660
C	7.30730	-5.98260	2.06080
O	7.40740	-7.26970	2.41450
C	6.25350	-8.12850	2.18300
O	6.31250	-5.48430	1.56200
O	8.38290	-1.70560	1.53350
H	9.67870	-1.63030	-0.77540
H	8.17590	-2.07810	-1.20270
H	10.13870	-3.82350	0.14480
H	8.50860	-4.29570	-0.31210
H	8.12120	-3.38710	3.25450
H	9.34990	-5.54650	1.60570
H	8.99450	-5.57690	3.32580
H	6.52100	-9.08880	2.62410
H	5.37290	-7.71000	2.67460
H	6.07590	-8.23260	1.11020

66. GGMe_Cis_WP_Conf_3

N	9.13350	-2.44200	-1.06200
C	9.10720	-3.44650	0.00330
C	8.61400	-2.91810	1.36250
N	8.45960	-3.79590	2.38420
C	8.64200	-5.23700	2.35860
C	7.39600	-6.08320	2.08210
O	6.35060	-5.39190	1.63830
C	5.13070	-6.13330	1.33960
O	7.40040	-7.29670	2.24630
O	8.38290	-1.70550	1.53320
H	9.70720	-1.64710	-0.77180
H	8.19420	-2.06120	-1.19930
H	10.11870	-3.85420	0.13890
H	8.47700	-4.28570	-0.31420
H	8.12870	-3.38780	3.25740
H	9.02920	-5.56360	3.32980
H	9.39010	-5.52620	1.61230
H	4.45250	-5.39760	0.90800
H	5.34210	-6.93260	0.62650
H	4.71680	-6.54480	2.26320

67. GGMe_Cis_WP_Conf_4

N	9.25010	-2.41730	-1.02950
C	9.05800	-3.45260	-0.01140
C	8.61400	-2.91820	1.36250
N	8.45960	-3.79560	2.38410
C	8.72280	-5.22350	2.38200
C	10.09220	-5.67170	2.90100
O	10.94920	-4.67830	3.11930
C	12.27240	-5.03090	3.61860
O	10.34910	-6.85520	3.08100
O	8.38290	-1.70550	1.53330
H	9.93430	-1.73150	-0.70140
H	8.38150	-1.89280	-1.15520
H	9.99140	-4.01720	0.10520
H	8.30630	-4.17030	-0.36790
H	8.17780	-3.37890	3.27040
H	7.97690	-5.72660	3.00810
H	8.61450	-5.64280	1.37630
H	12.81990	-4.08940	3.65740
H	12.18450	-5.46830	4.61590
H	12.75620	-5.73370	2.93700

68. GGMe_Cis_WP_Conf_5

N	9.19420	-2.44900	-1.04180
C	9.07650	-3.46400	0.00770
C	8.61360	-2.91990	1.36480
N	8.46000	-3.79460	2.38220
C	8.67790	-5.23450	2.36800
C	8.36770	-5.78810	3.75260
O	8.55410	-7.10720	3.80800
C	8.28590	-7.76130	5.08320
O	7.99370	-5.10570	4.69360
O	8.38290	-1.70490	1.53290
H	9.83870	-1.71540	-0.73740
H	8.29440	-1.97850	-1.16480
H	10.04580	-3.96340	0.14190
H	8.37420	-4.24370	-0.31710
H	8.15230	-3.39670	3.26800
H	9.71640	-5.49640	2.12000
H	8.02800	-5.74690	1.64420
H	8.50200	-8.81590	4.91390
H	8.93960	-7.34950	5.85510
H	7.23870	-7.61850	5.35910

69. GGMe_Cis_WP_Conf_6

N	9.18940	-2.39450	-0.99680
C	9.12700	-3.45170	0.02390
C	8.61370	-2.91700	1.36280
N	8.45970	-3.79770	2.38480
C	8.64610	-5.23650	2.34780
C	7.33130	-6.01890	2.32100
O	7.55930	-7.31080	2.05700
C	6.41920	-8.21830	2.06340
O	6.22750	-5.54710	2.53820
O	8.38310	-1.70480	1.53230
H	9.66550	-2.77450	-1.81840
H	9.78080	-1.62980	-0.66400
H	10.10510	-3.92400	0.20800
H	8.45440	-4.24380	-0.33050
H	8.14010	-3.39040	3.26250
H	9.19650	-5.56290	3.24100
H	9.24900	-5.53430	1.48710
H	6.81920	-9.17850	1.73730
H	6.01390	-8.29360	3.07510
H	5.65220	-7.86410	1.37190

70. GGMe_Cis_WP_Conf_7

N	9.19120	-2.39500	-0.99700
C	9.02570	-3.46770	-0.00470
C	8.61380	-2.91690	1.36250
N	8.45960	-3.79770	2.38500
C	8.71520	-5.22620	2.36790
C	10.00910	-5.62240	3.08180
O	10.31100	-6.90140	2.82840
C	11.47380	-7.47200	3.49700
O	10.66330	-4.89410	3.80930
O	8.38300	-1.70490	1.53240
H	9.34450	-2.82920	-1.91030
H	8.31800	-1.87040	-1.08460
H	9.97850	-4.00380	0.09540
H	8.27140	-4.21230	-0.30460
H	8.16430	-3.38580	3.26910
H	8.74560	-5.60930	1.34570
H	7.89640	-5.75600	2.87490
H	11.29080	-7.52450	4.57280
H	11.57990	-8.47220	3.07670
H	12.36050	-6.86990	3.28980

71. GGMe_Cis_WP_Conf_8

N	9.18710	-2.45920	-1.04710
C	9.07750	-3.46700	0.00960
C	8.61340	-2.91920	1.36510
N	8.46000	-3.79580	2.38260
C	8.68980	-5.23650	2.34240
C	8.40870	-5.92150	3.67270
O	7.99030	-5.08810	4.62260
C	7.68890	-5.63380	5.93830
O	8.55980	-7.12500	3.82460
O	8.38300	-1.70440	1.53220
H	9.82470	-1.71700	-0.75000
H	8.28300	-1.99930	-1.17700
H	10.05000	-3.96010	0.14520
H	8.38050	-4.25380	-0.30960
H	8.15160	-3.39710	3.26590
H	9.73040	-5.47760	2.08280
H	8.04900	-5.73160	1.59860
H	6.88970	-6.37400	5.85660
H	8.58730	-6.08580	6.36470
H	7.36620	-4.77660	6.52970

72. GGMe_Cis_WP_Conf_9

N	8.97140	-2.48700	-1.06300
C	9.08990	-3.47410	0.02140
C	8.61330	-2.91670	1.36420
N	8.45990	-3.79860	2.38440
C	8.61740	-5.24180	2.32010
C	7.47840	-6.03180	1.66790
O	6.41990	-5.29480	1.34210
C	5.30820	-5.96250	0.67850
O	7.56590	-7.23720	1.47310
O	8.38330	-1.70410	1.53130
H	7.99580	-2.19040	-1.15140
H	9.19130	-2.96160	-1.94220
H	10.14660	-3.75860	0.13470
H	8.54240	-4.40030	-0.19660
H	8.11840	-3.40240	3.25850
H	8.72010	-5.62570	3.34230
H	9.53580	-5.52250	1.79190
H	4.56090	-5.18320	0.53010
H	5.63950	-6.36740	-0.28090
H	4.91680	-6.76030	1.31330

73. GGMe_Cis_WP_Conf_10

N	9.45780	-2.41240	-0.92500
C	9.06170	-3.47550	0.01180
C	8.61330	-2.91640	1.36420
N	8.45990	-3.79900	2.38460
C	8.76660	-5.22010	2.36390
C	10.24870	-5.60510	2.42510
O	11.07050	-4.57810	2.62420
C	12.50200	-4.84860	2.64340
O	10.61560	-6.76540	2.29350
O	8.38330	-1.70410	1.53110
H	9.84620	-2.85910	-1.75940
H	10.22940	-1.87330	-0.52330
H	9.86340	-4.20730	0.17370
H	8.21580	-4.03460	-0.41470
H	8.17760	-3.39410	3.27550
H	8.35170	-5.70900	1.47510
H	8.28340	-5.69020	3.22890
H	12.81620	-5.24330	1.67410
H	12.96780	-3.88210	2.83480
H	12.73980	-5.55840	3.43850

74. GGMe_Cis_WP_Conf_11

N	8.91030	-2.52320	-1.08290
C	9.09970	-3.47360	0.02310
C	8.61310	-2.91560	1.36420
N	8.46000	-3.79990	2.38500
C	8.60830	-5.24510	2.29740
C	7.44210	-5.92130	1.56600
O	7.83850	-7.03920	0.94810
C	6.84090	-7.77940	0.18540
O	6.29790	-5.49750	1.54530
O	8.38340	-1.70390	1.53070
H	7.91080	-2.34130	-1.20830
H	9.21010	-2.98450	-1.94550
H	10.17250	-3.69260	0.13060
H	8.61020	-4.43650	-0.17100
H	8.11360	-3.40760	3.25860
H	8.63820	-5.65190	3.31640
H	9.54940	-5.52410	1.81470
H	6.05520	-8.14530	0.84960
H	6.41510	-7.13520	-0.58730
H	7.38550	-8.60970	-0.26400

75. GGMe_Cis_WP_Conf_12

N	9.48490	-2.43210	-0.92340
C	9.05330	-3.48160	0.01120
C	8.61300	-2.91550	1.36450
N	8.46000	-3.80020	2.38490
C	8.77870	-5.21980	2.34470
C	10.28760	-5.49490	2.35020
O	10.57650	-6.62810	1.70090
C	11.98000	-7.00870	1.59820
O	11.12210	-4.77600	2.87530
O	8.38340	-1.70380	1.53040
H	9.81240	-2.89140	-1.77700
H	10.30550	-1.95310	-0.54290
H	9.83160	-4.23920	0.16930
H	8.19090	-4.01380	-0.41700
H	8.18620	-3.39850	3.27970
H	8.35490	-5.69400	3.23920
H	8.32570	-5.70980	1.47750
H	11.98350	-7.91910	0.99900
H	12.54090	-6.21610	1.09760
H	12.39240	-7.19630	2.59170

76. GGMe_Cis_WP_Conf_13

N	10.20230	-2.74370	-0.55260
C	9.01650	-3.44690	-0.01940
C	8.61370	-2.91730	1.36310
N	8.45970	-3.79760	2.38460
C	8.86420	-5.19530	2.40550
C	10.38180	-5.37540	2.31110
O	10.70090	-6.65220	2.07430
C	12.11710	-6.97680	1.95720
O	11.19790	-4.47600	2.42420
O	8.38300	-1.70450	1.53220
H	10.37630	-3.08860	-1.50010
H	11.03310	-3.00740	-0.01700
H	9.13500	-4.53530	-0.01450
H	8.16250	-3.23070	-0.67320
H	8.17910	-3.38300	3.27270
H	8.38530	-5.77720	1.61040
H	8.53300	-5.63420	3.35450
H	12.14700	-8.03080	1.68210
H	12.57630	-6.36120	1.18100
H	12.61530	-6.81170	2.91490

77. GGMe_Cis_WP_Conf_14

N	10.54400	-3.33270	-0.14880
C	9.07430	-3.44780	0.00290
C	8.61340	-2.92030	1.36580
N	8.46020	-3.79560	2.38200
C	8.71940	-5.23040	2.35680
C	8.42990	-5.83020	3.72340
O	8.77760	-7.11700	3.75630
C	8.54040	-7.85560	4.99000
O	7.93870	-5.21930	4.65930
O	8.38290	-1.70350	1.53210
H	11.01860	-4.08170	0.36060
H	10.77780	-3.49130	-1.13180
H	8.70130	-4.46640	-0.16170
H	8.60140	-2.80190	-0.74120
H	8.13340	-3.40720	3.26640
H	9.76330	-5.45870	2.10500
H	8.07750	-5.75020	1.63160
H	7.46530	-7.96310	5.15170
H	9.00570	-8.82820	4.83010
H	9.00310	-7.33750	5.83200

78. GGA_m_trans_GP_Conf_1

N	8.16300	-4.43760	-0.04020
C	8.93950	-3.45090	0.71820
C	10.40840	-3.38240	0.29070
N	10.82700	-4.38480	-0.50970
C	12.21150	-4.54230	-0.94090
C	12.60940	-3.64640	-2.13010
N	12.59090	-2.31610	-1.87430
C	12.92480	-1.33910	-2.89940
O	12.93520	-4.12910	-3.21480
O	11.13920	-2.46440	0.68510
H	7.70060	-4.01890	-0.84150
H	8.94440	-3.72870	1.77790
H	8.54660	-2.42800	0.66530
H	10.11810	-5.05900	-0.77940
H	12.36070	-5.57430	-1.25800
H	12.86730	-4.32980	-0.08890
H	12.87330	-0.34090	-2.46050
H	13.93480	-1.51170	-3.28380
H	12.22980	-1.39750	-3.74410
H	12.27910	-2.01390	-0.95490
H	7.45060	-4.87890	0.53070

79. GGA_m_trans_GP_Conf_2

N	8.14550	-4.37710	-0.12190
C	8.92090	-3.40360	0.65290
C	10.40250	-3.36830	0.27040
N	10.82170	-4.37300	-0.52710
C	12.19160	-4.49310	-1.01230
C	13.17780	-5.10830	-0.00020
N	13.34760	-4.39280	1.13810
C	14.24320	-4.83880	2.19410
O	13.76540	-6.16290	-0.24040
O	11.14440	-2.47670	0.70290
H	7.73530	-3.95920	-0.95160
H	8.88680	-3.67760	1.71300
H	8.55540	-2.37090	0.58630
H	10.12420	-5.07260	-0.75940
H	12.54340	-3.49540	-1.29850
H	12.19490	-5.13770	-1.89120
H	14.04300	-4.25570	3.09530
H	14.08030	-5.89930	2.40460
H	15.29440	-4.70930	1.91150
H	12.83050	-3.52260	1.23380
H	7.39270	-4.78140	0.42410

80. GGA_m_trans_GP_Conf_3

N	8.28590	-4.70970	0.36780
C	8.93530	-3.43850	0.70260
C	10.41070	-3.38750	0.29800
N	10.82900	-4.38930	-0.50330
C	12.20380	-4.52530	-0.97050
C	12.56980	-3.63050	-2.17100
N	12.46570	-2.29850	-1.94500
C	12.78220	-1.32100	-2.97480
O	12.94350	-4.11810	-3.23780
O	11.13710	-2.46010	0.67860
H	7.30980	-4.58290	0.12400
H	8.89290	-3.17020	1.76600
H	8.44210	-2.62650	0.15730
H	10.11590	-5.05370	-0.78650
H	12.36330	-5.55640	-1.28570
H	12.87620	-4.29910	-0.13500
H	12.34820	-1.62930	-3.92950
H	12.36760	-0.35390	-2.68310
H	13.86480	-1.21760	-3.11440
H	12.17890	-1.99570	-1.01740
H	8.32860	-5.37040	1.13790

81. GGA_m_trans_GP_Conf_4

N	8.25820	-4.66000	0.28840
C	8.91630	-3.39650	0.63630
C	10.40500	-3.37400	0.27780
N	10.82430	-4.37760	-0.52070
C	12.18040	-4.47190	-1.04900
C	13.21500	-5.05500	-0.06660
N	13.38620	-4.34060	1.07250
C	14.34430	-4.74040	2.09140
O	13.83530	-6.08480	-0.33080
O	11.14210	-2.47190	0.69630
H	7.29710	-4.51920	-0.00210
H	8.84220	-3.12360	1.69630
H	8.45550	-2.57920	0.07090
H	10.12140	-5.06710	-0.76660
H	12.50300	-3.47080	-1.35770
H	12.16880	-5.12580	-1.92080
H	15.37160	-4.48650	1.80380
H	14.10120	-4.23040	3.02610
H	14.29490	-5.82130	2.24400
H	12.85600	-3.47880	1.17540
H	8.25280	-5.31020	1.06850

82. GGA_m_trans_GP_Conf_5

N	8.12650	-4.35450	-0.04100
C	8.93380	-3.40750	0.73130
C	10.40260	-3.36410	0.29720
N	10.80370	-4.37590	-0.50470
C	12.16270	-4.47230	-0.97510
C	12.30240	-5.68940	-1.89110
N	13.55400	-5.90570	-2.37480
C	13.84840	-7.02250	-3.26430
O	11.35040	-6.41490	-2.17060
O	11.15280	-2.46630	0.68700
H	7.74930	-3.93180	-0.88390
H	8.93560	-3.71800	1.78210
H	8.57300	-2.37060	0.71220
H	10.13370	-5.08430	-0.79280
H	12.86070	-4.55550	-0.13070
H	12.44640	-3.56140	-1.52000
H	14.90500	-6.98460	-3.53490
H	13.63640	-7.97750	-2.77410
H	13.24200	-6.96380	-4.17290
H	14.30060	-5.28280	-2.10420
H	7.34840	-4.71630	0.49920

83. GGAm_trans_GP_Conf_6

N	8.48630	-2.27750	1.57570
C	8.90890	-3.37720	0.72720
C	10.39150	-3.35140	0.30940
N	10.78580	-4.37110	-0.49740
C	12.14360	-4.49120	-0.97350
C	12.24660	-5.73930	-1.85350
N	13.47310	-5.98420	-2.37770
C	13.72460	-7.13630	-3.23590
O	11.27620	-6.46640	-2.06550
O	11.16610	-2.46940	0.68130
H	8.66480	-1.39330	1.10540
H	8.29050	-3.38890	-0.17950
H	8.71000	-4.32510	1.24370
H	10.14940	-5.09870	-0.80640
H	12.84560	-4.56480	-0.13200
H	12.43460	-3.60090	-1.54680
H	14.77510	-7.12870	-3.53120
H	13.50580	-8.06840	-2.70690
H	13.09830	-7.09650	-4.13200
H	14.23180	-5.35190	-2.16900
H	9.05710	-2.25550	2.41740

84. GGA_m_trans_GP_Conf_7

N	8.52080	-2.55290	1.78040
C	8.88250	-3.30260	0.59120
C	10.38600	-3.34810	0.27810
N	10.79960	-4.36340	-0.52520
C	12.16960	-4.47450	-1.02540
C	13.14030	-5.12850	-0.02340
N	13.43840	-4.36470	1.05680
C	14.29390	-4.85030	2.12860
O	13.60400	-6.25060	-0.22360
O	11.16220	-2.48550	0.70180
H	8.96500	-1.63800	1.75270
H	8.39050	-2.84510	-0.27790
H	8.48350	-4.32100	0.67080
H	10.14500	-5.09360	-0.76790
H	12.51800	-3.47060	-1.28790
H	12.16340	-5.09850	-1.91910
H	13.75510	-5.51950	2.81080
H	15.13210	-5.40520	1.70200
H	14.67430	-3.99690	2.69390
H	12.93140	-3.49100	1.16670
H	8.87260	-3.01680	2.61410

85. GGA_m_trans_GP_Conf_8

N	8.37140	-2.20960	1.26690
C	8.95270	-3.46730	0.83350
C	10.39890	-3.37810	0.32220
N	10.81060	-4.38920	-0.48730
C	12.19070	-4.52430	-0.95270
C	12.51140	-3.66190	-2.18850
N	12.56350	-2.32800	-1.94990
C	12.79820	-1.36560	-3.01540
O	12.71470	-4.17390	-3.28880
O	11.15090	-2.45920	0.66320
H	8.25080	-1.58210	0.47590
H	8.30970	-3.91760	0.06790
H	8.95810	-4.16470	1.68220
H	10.13230	-5.06410	-0.81130
H	12.36200	-5.56340	-1.23400
H	12.85590	-4.25950	-0.12470
H	13.13700	-0.42490	-2.57610
H	13.56730	-1.74870	-3.68920
H	11.89200	-1.17890	-3.60490
H	12.29350	-2.00690	-1.02440
H	9.00990	-1.74380	1.90760

86. GGA_m_trans_GP_Conf_9

N	8.41240	-2.16050	1.31580
C	8.89410	-3.35880	0.65640
C	10.38720	-3.35030	0.28180
N	10.80100	-4.36570	-0.52240
C	12.18610	-4.51370	-0.96810
C	13.09810	-5.18690	0.07480
N	13.38660	-4.41780	1.15440
C	14.18250	-4.91900	2.26460
O	13.52520	-6.32890	-0.09120
O	11.16110	-2.48320	0.69880
H	8.50790	-1.35740	0.69970
H	8.29640	-3.53810	-0.24560
H	8.72320	-4.22080	1.31560
H	10.14340	-5.09140	-0.77140
H	12.56850	-3.52000	-1.22170
H	12.19850	-5.14150	-1.85910
H	15.00940	-5.51770	1.87730
H	14.58050	-4.07220	2.82770
H	13.59170	-5.55080	2.93940
H	12.90970	-3.52430	1.23390
H	8.98930	-1.95830	2.12860

87. GGA_m_trans_GP_Conf_10

N	8.55100	-2.48390	1.79530
C	8.92500	-3.43050	0.76280
C	10.39800	-3.37540	0.31910
N	10.81010	-4.38730	-0.49040
C	12.17460	-4.48490	-1.00790
C	12.41910	-3.61380	-2.25420
N	12.47000	-2.28020	-2.01050
C	12.62680	-1.30810	-3.08180
O	12.56290	-4.11620	-3.36830
O	11.15170	-2.46120	0.66620
H	8.79910	-1.54100	1.50630
H	8.30450	-3.25130	-0.12580
H	8.68820	-4.44630	1.10260
H	10.13290	-5.06670	-0.80820
H	12.36410	-5.51920	-1.29490
H	12.86170	-4.20110	-0.20480
H	12.99250	-0.36960	-2.65980
H	13.34850	-1.68410	-3.80980
H	11.68130	-1.12010	-3.60560
H	12.24660	-1.96700	-1.07030
H	9.07930	-2.66310	2.64540

88. GGA_m_trans_GP_Conf_11

N	8.05350	-4.47820	0.38040
C	8.93860	-3.40320	0.78880
C	10.39900	-3.37780	0.31380
N	10.81230	-4.38620	-0.49300
C	12.18460	-4.49380	-0.98330
C	12.46280	-3.61560	-2.21830
N	12.50110	-2.28390	-1.96740
C	12.69760	-1.30790	-3.02830
O	12.64310	-4.11370	-3.32930
O	11.15020	-2.46210	0.66890
H	8.31400	-5.39690	0.71790
H	8.98060	-3.36750	1.88300
H	8.50380	-2.44660	0.47920
H	10.13130	-5.06440	-0.80300
H	12.37030	-5.52750	-1.27520
H	12.85940	-4.22090	-0.16570
H	13.46540	-1.66680	-3.71710
H	11.77860	-1.13770	-3.60280
H	13.02020	-0.36320	-2.58580
H	12.25090	-1.97630	-1.03120
H	7.83280	-4.49800	-0.60800

89. GGA_m_trans_GP_Conf_12

N	7.99380	-4.33850	0.17390
C	8.90260	-3.31940	0.66480
C	10.38930	-3.35520	0.28040
N	10.80400	-4.36680	-0.52160
C	12.18400	-4.49240	-0.98510
C	13.11730	-5.15220	0.04820
N	13.39820	-4.38240	1.12830
C	14.21800	-4.87030	2.22670
O	13.56510	-6.28540	-0.12670
O	11.15860	-2.48190	0.69810
H	8.16300	-5.27060	0.53220
H	8.87410	-3.31400	1.75990
H	8.53860	-2.33330	0.35570
H	10.14080	-5.08670	-0.77010
H	12.54890	-3.49220	-1.23980
H	12.19650	-5.11950	-1.87660
H	14.58370	-4.01750	2.80230
H	13.65520	-5.53590	2.89290
H	15.06710	-5.42970	1.82810
H	12.90340	-3.49850	1.21480
H	7.86570	-4.34780	-0.83080

90. GGAm_cis_GP_Conf_1

N	7.33710	-5.12210	0.17010
C	7.47250	-6.46180	0.71120
C	8.19910	-7.45880	-0.21020
N	8.22980	-8.77840	0.17840
C	7.70280	-9.35650	1.40580
C	6.28240	-9.94620	1.34230
N	5.68040	-9.94850	0.12750
C	4.33740	-10.47750	-0.06800
O	5.76840	-10.39570	2.36320
O	8.73600	-7.09970	-1.25350
H	8.24470	-4.78710	-0.14440
H	8.02730	-6.40800	1.65790
H	6.47870	-6.84810	0.96570
H	8.80370	-9.36200	-0.41900
H	7.70330	-8.62380	2.21590
H	8.36290	-10.16650	1.73040
H	4.19970	-10.72150	-1.12330
H	4.21230	-11.38000	0.53400
H	3.57140	-9.75510	0.23610
H	6.17620	-9.53370	-0.64870
H	6.74970	-5.13890	-0.65990

91. GGA_m_cis_GP_Conf_2

N	7.34230	-5.12090	0.17460
C	7.28040	-6.51040	0.58820
C	8.16390	-7.46760	-0.23260
N	8.26770	-8.76880	0.20250
C	7.59290	-9.38280	1.33650
C	8.36040	-9.40820	2.67060
N	9.63260	-8.93990	2.64710
C	10.46680	-8.90960	3.84080
O	7.81310	-9.85650	3.67450
O	8.75560	-7.09500	-1.24090
H	8.27930	-4.75410	0.32140
H	7.54370	-6.58080	1.65010
H	6.24110	-6.85790	0.51130
H	8.78140	-9.36750	-0.43330
H	7.35950	-10.42320	1.09080
H	6.63490	-8.89650	1.53340
H	10.29450	-9.81530	4.42590
H	11.51610	-8.86280	3.54240
H	10.23480	-8.04500	4.47320
H	9.98510	-8.56720	1.77700
H	7.17600	-5.05410	-0.82680

92. GGAm_cis_GP_Conf_3

N	7.31140	-5.13150	0.20390
C	7.36920	-6.50660	0.66700
C	8.18320	-7.46190	-0.22590
N	8.25680	-8.76440	0.17600
C	7.65000	-9.35260	1.34710
C	8.00850	-10.84660	1.39150
N	7.50210	-11.53010	2.44970
C	7.77370	-12.94960	2.64750
O	8.69450	-11.37430	0.52120
O	8.73870	-7.06750	-1.24810
H	6.91750	-5.10690	-0.73400
H	6.34570	-6.89370	0.76080
H	7.79130	-6.52330	1.68080
H	8.78990	-9.40520	-0.40630
H	6.55440	-9.25790	1.33450
H	8.00520	-8.88000	2.27460
H	8.80270	-13.11850	2.98290
H	7.08240	-13.33920	3.39700
H	7.62720	-13.48630	1.70780
H	6.98840	-11.02840	3.15940
H	8.25700	-4.76930	0.10270

93. GGAm_cis_GP_Conf_4

N	5.92480	-6.57690	0.07080
C	7.31430	-6.48740	0.56750
C	8.17430	-7.47410	-0.22600
N	8.25540	-8.76920	0.19980
C	7.55330	-9.44720	1.28320
C	6.31890	-10.26580	0.84380
N	5.32240	-9.56390	0.25840
C	4.11530	-10.22730	-0.21240
O	6.27550	-11.48040	1.04440
O	8.75200	-7.09860	-1.24510
H	5.89520	-6.26650	-0.89900
H	7.31040	-6.70750	1.63850
H	7.76910	-5.50110	0.42090
H	8.78690	-9.35700	-0.43300
H	7.25770	-8.71620	2.03990
H	8.23430	-10.15800	1.75570
H	3.44430	-9.47410	-0.63080
H	4.34880	-10.96790	-0.98430
H	3.60830	-10.74640	0.60730
H	5.41850	-8.55120	0.14530
H	5.32230	-5.94980	0.59890

94. GGA_m_cis_GP_Conf_5

N	8.40290	-5.96200	1.69780
C	7.46390	-6.45010	0.66530
C	8.19140	-7.46960	-0.21510
N	8.23720	-8.77370	0.18760
C	7.77980	-9.38720	1.42900
C	8.89570	-9.63050	2.46900
N	9.49300	-8.52070	2.95940
C	10.58190	-8.61660	3.92030
O	9.18810	-10.77630	2.81370
O	8.74230	-7.10040	-1.25130
H	7.93320	-5.30220	2.31370
H	7.11020	-5.66400	-0.01120
H	6.59590	-6.88450	1.16930
H	8.79770	-9.35530	-0.42550
H	7.35410	-10.36740	1.20460
H	6.99160	-8.77210	1.86980
H	10.86990	-7.60780	4.22330
H	10.27110	-9.18330	4.80330
H	11.45130	-9.12240	3.48630
H	9.19830	-7.60180	2.61860
H	9.16130	-5.45290	1.24650

95. GGA_m_cis_GP_Conf_6

N	7.66910	-5.11090	0.24280
C	7.44340	-6.47740	0.68620
C	8.19790	-7.46040	-0.21000
N	8.23060	-8.77770	0.17940
C	7.64290	-9.37370	1.36840
C	6.20250	-9.90220	1.24320
N	5.65840	-9.89520	0.00080
C	4.30310	-10.36450	-0.25260
O	5.62440	-10.32150	2.24240
O	8.73710	-7.10200	-1.25300
H	8.00150	-5.11230	-0.71890
H	6.38240	-6.77860	0.67780
H	7.78810	-6.60290	1.72200
H	8.80300	-9.35890	-0.42070
H	7.64870	-8.66950	2.20360
H	8.26140	-10.22050	1.68060
H	4.21380	-10.65300	-1.30190
H	4.09790	-11.22900	0.38170
H	3.55900	-9.59130	-0.02880
H	6.19920	-9.49590	-0.75320
H	6.83080	-4.54600	0.31050

96. GGA_m_cis_GP_Conf_7

N	8.26270	-6.23490	1.92290
C	7.47930	-6.46290	0.70020
C	8.20190	-7.46180	-0.20920
N	8.22700	-8.77880	0.17850
C	7.74440	-9.34040	1.43400
C	6.33020	-9.94000	1.42110
N	5.67110	-9.90840	0.23250
C	4.33120	-10.44600	0.05520
O	5.86490	-10.40970	2.45680
O	8.73530	-7.09940	-1.25480
H	7.75050	-5.64360	2.57150
H	7.31370	-5.56710	0.08920
H	6.50110	-6.86170	0.99260
H	8.80440	-9.35890	-0.41870
H	7.78270	-8.57910	2.21690
H	8.42100	-10.14080	1.74820
H	4.33230	-11.27670	-0.65870
H	3.98710	-10.81060	1.02400
H	3.64380	-9.67190	-0.30210
H	6.16010	-9.51520	-0.55970
H	9.13490	-5.76000	1.70380

97. GGAm_cis_GP_Conf_8

N	5.86730	-6.83800	0.38330
C	7.28740	-6.51160	0.57730
C	8.16290	-7.47170	-0.23420
N	8.26890	-8.76820	0.20540
C	7.53820	-9.39190	1.30160
C	8.25380	-9.45160	2.65970
N	9.51450	-8.94470	2.70130
C	10.32610	-8.93690	3.90840
O	7.67390	-9.94230	3.62550
O	8.75710	-7.09400	-1.24090
H	5.28260	-6.26550	0.98570
H	7.51530	-6.60750	1.64510
H	7.57270	-5.50210	0.25680
H	8.77970	-9.36500	-0.43460
H	7.30010	-10.42410	1.02760
H	6.58220	-8.88220	1.44460
H	11.24090	-9.52290	3.76950
H	10.59900	-7.91440	4.19070
H	9.73560	-9.38340	4.70960
H	9.89710	-8.58010	1.83980
H	5.58720	-6.65210	-0.57650

98. GGAm_cis_GP_Conf_9

N	8.00550	-6.34300	1.98040
C	7.38450	-6.49360	0.65240
C	8.18300	-7.46600	-0.22500
N	8.25570	-8.76400	0.17860
C	7.61520	-9.36600	1.32890
C	8.24460	-10.73920	1.58250
N	7.98090	-11.28060	2.80040
C	8.47890	-12.59820	3.17690
O	8.90220	-11.32150	0.72320
O	8.74030	-7.07100	-1.24860
H	8.93620	-5.94230	1.88630
H	7.31570	-5.56290	0.07710
H	6.36730	-6.87960	0.79710
H	8.78960	-9.39790	-0.40940
H	6.53820	-9.52740	1.15850
H	7.72520	-8.71330	2.20140
H	8.00040	-12.90140	4.11000
H	8.23830	-13.32360	2.39610
H	9.56560	-12.59160	3.31380
H	7.52100	-10.71350	3.49720
H	7.46390	-5.69780	2.54990

99. GGAm_cis_GP_Conf_10

N	5.94820	-6.86080	0.66420
C	7.37570	-6.49560	0.64650
C	8.18500	-7.46550	-0.22360
N	8.25350	-8.76450	0.17720
C	7.69030	-9.34700	1.37710
C	7.70910	-10.87270	1.24190
N	6.92140	-11.54140	2.12410
C	6.86100	-12.99800	2.14570
O	8.42310	-11.44370	0.42090
O	8.73920	-7.07140	-1.24930
H	5.55960	-6.79270	-0.27390
H	7.74630	-6.53150	1.67900
H	7.58190	-5.49580	0.24670
H	8.79090	-9.39740	-0.40860
H	6.67140	-8.97570	1.52900
H	8.28230	-9.09220	2.27130
H	6.36430	-13.39100	1.25210
H	7.87130	-13.41210	2.18390
H	6.30870	-13.31360	3.03280
H	6.28440	-11.01630	2.70480
H	5.42680	-6.21020	1.24620

100.	GGAm_cis_GP_Conf_11		
N	7.19620	-5.16200	0.05100
C	7.29420	-6.50600	0.59430
C	8.15430	-7.47150	-0.23850
N	8.27730	-8.76650	0.21060
C	7.47610	-9.41340	1.22370
C	6.09880	-9.89530	0.71950
N	5.58070	-10.96150	1.38710
C	4.24860	-11.47640	1.08890
O	5.50460	-9.32680	-0.18960
O	8.76180	-7.09850	-1.23650
H	8.12370	-4.83240	-0.20780
H	6.28770	-6.92400	0.69340
H	7.72100	-6.45290	1.60630
H	8.77520	-9.36250	-0.43990
H	7.29980	-8.72150	2.05430
H	8.04840	-10.25170	1.63720
H	4.17860	-11.77630	0.03950
H	4.05670	-12.34240	1.72480
H	3.48600	-10.71450	1.27720
H	6.12500	-11.40500	2.11170
H	6.66630	-5.18550	-0.81680

101.	GGAm_cis_GP_Conf_12		
N	7.50970	-5.08300	0.25080
C	7.46260	-6.46340	0.70190
C	8.20910	-7.45760	-0.20340
N	8.21840	-8.78140	0.17290
C	7.84670	-9.31970	1.46090
C	8.94320	-9.17810	2.53830
N	8.91300	-10.11980	3.51990
C	9.82730	-10.06940	4.65570
O	9.75180	-8.25690	2.52470
O	8.73120	-7.10620	-1.25610
H	8.46150	-4.73340	0.33040
H	6.41260	-6.78240	0.76880
H	7.87960	-6.52190	1.71190
H	8.81000	-9.35380	-0.41770
H	7.56870	-10.37200	1.33140
H	6.95190	-8.80840	1.83170
H	9.62370	-10.92040	5.30790
H	10.86620	-10.11470	4.31680
H	9.69310	-9.14190	5.22020
H	8.24270	-10.87190	3.46520
H	7.29000	-5.04350	-0.74220

102. GGAm_cis_GP_Conf_13

N	6.04920	-6.82250	0.85210
C	7.46020	-6.45450	0.67720
C	8.19870	-7.46290	-0.20850
N	8.22730	-8.77900	0.18320
C	7.81530	-9.36510	1.45070
C	6.70560	-10.42460	1.37360
N	6.07620	-10.55560	0.17930
C	4.94870	-11.45660	-0.00340
O	6.44870	-11.10420	2.36470
O	8.73860	-7.10800	-1.25360
H	5.61550	-6.25620	1.57570
H	7.93450	-6.43230	1.66600
H	7.62700	-5.47730	0.20880
H	8.80420	-9.34910	-0.42540
H	7.44460	-8.58470	2.11410
H	8.66750	-9.84310	1.94590
H	5.11120	-12.35030	0.60150
H	4.00390	-10.99690	0.31160
H	4.87710	-11.73850	-1.05650
H	6.27690	-9.86010	-0.52540
H	5.52880	-6.65820	-0.00590

103. GGAm_cis_GP_Conf_14

N	7.79200	-6.38380	1.96770
C	7.31340	-6.49170	0.58350
C	8.16420	-7.47160	-0.23060
N	8.26430	-8.76960	0.20690
C	7.51130	-9.44140	1.25630
C	8.33850	-10.01320	2.41770
N	9.64600	-9.65510	2.46290
C	10.51660	-10.05220	3.55850
O	7.80250	-10.76400	3.22960
O	8.75780	-7.10310	-1.24130
H	8.66730	-5.86760	2.00320
H	6.27700	-6.85040	0.60540
H	7.32630	-5.55310	0.01680
H	8.78230	-9.35470	-0.43930
H	6.93890	-10.27790	0.84110
H	6.80140	-8.74620	1.70270
H	10.24140	-11.05820	3.87970
H	11.55390	-10.05120	3.21560
H	10.42120	-9.37960	4.41980
H	9.94780	-8.93340	1.82360
H	7.12450	-5.87670	2.54190

104. GGA_m_cis_GP_Conf_15

N	6.27780	-5.81760	-0.25150
C	7.30570	-6.46740	0.55740
C	8.15570	-7.46940	-0.23280
N	8.27100	-8.76950	0.21220
C	7.41350	-9.45700	1.15210
C	5.98960	-9.72030	0.61850
N	5.37110	-10.81600	1.13270
C	3.98320	-11.13650	0.81680
O	5.45020	-8.96740	-0.18700
O	8.76280	-7.10990	-1.23810
H	6.71250	-5.41100	-1.07700
H	6.82380	-6.91920	1.42680
H	7.99920	-5.70330	0.92810
H	8.77910	-9.35020	-0.44560
H	7.31750	-8.87680	2.07640
H	7.90110	-10.39770	1.42930
H	3.82760	-11.07660	-0.26260
H	3.76930	-12.15140	1.15670
H	3.29150	-10.43970	1.30240
H	5.86070	-11.38700	1.80580
H	5.62130	-6.52550	-0.57550

105. GGAm_cis_GP_Conf_16

N	8.32580	-5.30250	1.06150
C	7.47700	-6.42410	0.66700
C	8.20290	-7.45750	-0.20260
N	8.22030	-8.78230	0.17970
C	7.94570	-9.32260	1.49260
C	9.00820	-8.95830	2.55080
N	9.15410	-9.85780	3.55930
C	10.03540	-9.60570	4.69450
O	9.64550	-7.91080	2.49540
O	8.73640	-7.11660	-1.25500
H	8.74970	-4.89820	0.22920
H	6.64710	-6.04280	0.06040
H	7.04620	-6.86260	1.56940
H	8.80900	-9.34260	-0.42650
H	7.85310	-10.40980	1.39840
H	6.97800	-8.96250	1.85880
H	11.01470	-9.27940	4.33710
H	9.63110	-8.82510	5.34780
H	10.14850	-10.52940	5.26480
H	8.59070	-10.69520	3.55750
H	9.08360	-5.65550	1.64320

106. GGAm_cis_GP_Conf_17

N	6.09280	-6.82660	0.96530
C	7.49030	-6.44830	0.69260
C	8.20400	-7.46210	-0.20490
N	8.22230	-8.77950	0.17800
C	7.83810	-9.32730	1.46130
C	8.92180	-9.19160	2.54430
N	8.95340	-10.19720	3.46220
C	9.85000	-10.15820	4.61100
O	9.67270	-8.22210	2.60080
O	8.73530	-7.10900	-1.25500
H	5.53970	-6.78550	0.11250
H	8.03040	-6.40460	1.64450
H	7.60600	-5.48220	0.18760
H	8.80700	-9.34840	-0.42240
H	7.55940	-10.37790	1.31960
H	6.94290	-8.79640	1.80410
H	10.88090	-10.00420	4.28140
H	9.58510	-9.34250	5.29190
H	9.78020	-11.10800	5.14440
H	8.31630	-10.97340	3.36530
H	5.67530	-6.17190	1.62120

107. GGA_m_cis_GP_Conf_18

N	7.67960	-6.42720	1.98090
C	7.28730	-6.49950	0.56270
C	8.15890	-7.47340	-0.23370
N	8.27080	-8.76720	0.20900
C	7.48110	-9.41760	1.23280
C	6.10700	-9.90380	0.74210
N	5.64590	-11.03790	1.33850
C	4.31530	-11.56400	1.05930
O	5.45490	-9.28600	-0.09480
O	8.76040	-7.10270	-1.23890
H	7.03510	-5.82980	2.49170
H	7.35430	-5.54560	0.02680
H	6.25210	-6.85300	0.50640
H	8.77850	-9.35560	-0.44070
H	7.32050	-8.70070	2.04590
H	8.06450	-10.25000	1.64330
H	4.20290	-12.52400	1.56660
H	3.53750	-10.87790	1.41040
H	4.18230	-11.70640	-0.01640
H	6.22590	-11.50950	2.01600
H	8.60440	-6.01370	2.07410

108. GGAm_cis_GP_Conf_19

N	6.42870	-6.74830	1.53020
C	7.53730	-6.36580	0.63720
C	8.19790	-7.46670	-0.20350
N	8.22360	-8.77870	0.18630
C	7.82290	-9.43120	1.43350
C	8.78380	-9.15720	2.60380
N	8.36000	-8.19010	3.45780
C	9.16390	-7.75700	4.59010
O	9.83500	-9.78090	2.73550
O	8.74160	-7.12460	-1.25280
H	6.07230	-5.91110	1.98680
H	8.33810	-5.94360	1.25720
H	7.26550	-5.59720	-0.09510
H	8.80550	-9.32900	-0.43430
H	7.85310	-10.50670	1.24890
H	6.80210	-9.15310	1.69420
H	9.62370	-8.62840	5.06080
H	9.96730	-7.07440	4.28630
H	8.52080	-7.25230	5.31480
H	7.53940	-7.65980	3.17390
H	5.65000	-7.12030	0.98950

109. GGAm_cis_GP_Conf_20

N	7.03980	-6.59350	1.92180
C	7.29010	-6.42790	0.47870
C	8.16160	-7.47580	-0.22680
N	8.26270	-8.76880	0.21130
C	7.54670	-9.50100	1.25690
C	6.09280	-9.83820	0.88210
N	5.17010	-8.99790	1.41750
C	3.75070	-9.12790	1.12730
O	5.81720	-10.79770	0.16460
O	8.76180	-7.11940	-1.23980
H	6.48260	-5.80700	2.24970
H	7.76120	-5.47220	0.22200
H	6.32120	-6.45150	-0.03580
H	8.78250	-9.33490	-0.44900
H	7.58940	-8.95360	2.19810
H	8.06540	-10.45280	1.38520
H	3.47730	-10.18510	1.12790
H	3.17760	-8.60620	1.89740
H	3.49260	-8.71310	0.14490
H	5.52760	-8.16910	1.88710
H	7.91460	-6.54720	2.44120

110.	GGAm_trans_WP_Conf_1		
N	8.06910	-4.49270	0.34170
C	8.95430	-3.42960	0.81950
C	10.39960	-3.38240	0.31400
N	10.81130	-4.38660	-0.49000
C	12.15050	-4.44720	-1.05280
C	13.21610	-5.08240	-0.15000
N	12.80550	-5.69240	0.96960
C	13.72450	-6.31820	1.91760
O	14.41590	-5.01160	-0.49240
O	11.15250	-2.45410	0.67060
H	8.39780	-5.42230	0.60800
H	9.02250	-3.47510	1.91430
H	8.51730	-2.45040	0.58830
H	10.12930	-5.06750	-0.80790
H	12.50080	-3.43890	-1.29850
H	12.11220	-5.02590	-1.98220
H	13.17030	-6.56260	2.82600
H	14.16010	-7.23510	1.50420
H	14.53630	-5.62890	2.16830
H	11.80960	-5.76000	1.14900
H	7.95160	-4.47350	-0.67290

111.	GGAm_trans_WP_Conf_2		
N	8.03310	-4.40720	0.22780
C	8.90220	-3.30930	0.64630
C	10.38970	-3.36060	0.28180
N	10.80330	-4.36760	-0.51760
C	12.18880	-4.52940	-0.92700
C	12.62310	-3.68400	-2.13120
N	11.66980	-3.06630	-2.84140
C	11.96000	-2.19090	-3.97490
O	13.83930	-3.61880	-2.41170
O	11.16120	-2.47320	0.69880
H	8.33570	-5.30870	0.59990
H	8.85760	-3.19190	1.73630
H	8.52590	-2.36500	0.23050
H	10.13850	-5.08930	-0.77630
H	12.35730	-5.58280	-1.17660
H	12.85680	-4.26740	-0.09970
H	12.63130	-2.68870	-4.67990
H	11.02080	-1.95430	-4.47820
H	12.43120	-1.26030	-3.63850
H	10.70180	-3.17440	-2.55670
H	7.96100	-4.48330	-0.78770

112.	GGAm_trans_WP_Conf_3		
N	8.24910	-4.69080	0.58240
C	8.94620	-3.41130	0.78170
C	10.40020	-3.38780	0.31320
N	10.81920	-4.38820	-0.49030
C	12.15920	-4.41160	-1.05980
C	13.26150	-4.95110	-0.13610
N	12.89140	-5.74970	0.87370
C	13.84590	-6.32400	1.82020
O	14.45240	-4.65270	-0.36940
O	11.14880	-2.45490	0.66830
H	7.24230	-4.54220	0.67780
H	8.96040	-3.06770	1.82510
H	8.43350	-2.63020	0.20520
H	10.12460	-5.05970	-0.80450
H	12.46350	-3.40120	-1.35150
H	12.14480	-5.03470	-1.96140
H	14.35630	-5.53580	2.38460
H	13.29940	-6.96320	2.51600
H	14.60150	-6.92170	1.29980
H	11.90910	-5.98240	0.97510
H	8.50120	-5.34750	1.32450

113. GGA_m_trans_WP_Conf_4

N	8.04400	-4.21890	-0.13220
C	8.91100	-3.33200	0.65850
C	10.38910	-3.36090	0.27210
N	10.81000	-4.36490	-0.52560
C	12.21060	-4.53300	-0.88510
C	12.70180	-3.67310	-2.05970
N	11.78270	-3.21780	-2.92150
C	12.11350	-2.38210	-4.07380
O	13.92660	-3.45950	-2.18590
O	11.15830	-2.47870	0.70420
H	7.79240	-3.77040	-1.01570
H	8.87090	-3.63680	1.71230
H	8.61290	-2.27510	0.63010
H	10.13530	-5.08610	-0.76390
H	12.38120	-5.58330	-1.14780
H	12.85060	-4.29040	-0.03070
H	12.33820	-1.35360	-3.76710
H	12.98350	-2.78570	-4.59880
H	11.25830	-2.37150	-4.75210
H	10.80790	-3.44700	-2.75700
H	7.16210	-4.35840	0.36520

114.	GGAm_trans_WP_Conf_5		
N	8.04090	-4.21230	-0.06340
C	8.94630	-3.41970	0.78380
C	10.39600	-3.37980	0.30230
N	10.81590	-4.38120	-0.49980
C	12.14890	-4.39840	-1.08340
C	13.28230	-4.88720	-0.17090
N	12.95540	-5.62400	0.89880
C	13.95420	-6.13610	1.83590
O	14.46300	-4.60700	-0.47150
O	11.15250	-2.46160	0.67810
H	7.80900	-3.68860	-0.91060
H	8.97060	-3.86250	1.78840
H	8.64190	-2.37240	0.90940
H	10.12830	-5.06810	-0.79390
H	12.42760	-3.39130	-1.41100
H	12.13260	-5.04650	-1.96740
H	13.44870	-6.75410	2.58000
H	14.70270	-6.74140	1.31430
H	14.46900	-5.31350	2.34510
H	11.97620	-5.83360	1.06410
H	7.15450	-4.34540	0.42860

115.	GGAm_trans_WP_Conf_6		
N	8.23260	-4.63820	0.58340
C	8.90740	-3.33200	0.64820
C	10.39080	-3.36720	0.28270
N	10.81180	-4.37020	-0.51660
C	12.21520	-4.56450	-0.85020
C	12.76860	-3.69910	-1.99060
N	11.89490	-3.12390	-2.82670
C	12.31410	-2.27920	-3.94460
O	14.00720	-3.58450	-2.11470
O	11.15680	-2.47300	0.69500
H	8.50460	-5.21000	1.38680
H	8.85090	-2.84520	1.63040
H	8.42930	-2.64970	-0.06750
H	10.13330	-5.08020	-0.77440
H	12.36310	-5.61370	-1.13080
H	12.83960	-4.36090	0.02620
H	12.84250	-1.39020	-3.58270
H	12.98090	-2.82710	-4.61860
H	11.42560	-1.96580	-4.49560
H	10.90370	-3.28690	-2.68180
H	7.22400	-4.49830	0.67610

116.	GGAm_trans_WP_Conf_7		
N	8.04990	-4.46180	0.25340
C	8.92090	-3.37870	0.71480
C	10.39650	-3.37390	0.29160
N	10.80020	-4.37130	-0.50150
C	12.14910	-4.53940	-1.00570
C	12.18450	-5.80760	-1.86370
N	13.36860	-6.12320	-2.40330
C	13.53590	-7.30590	-3.24810
O	11.15660	-6.49510	-2.03720
O	11.15920	-2.46280	0.68820
H	8.35910	-5.37970	0.57780
H	8.91910	-3.35170	1.81150
H	8.50730	-2.41580	0.39040
H	10.13690	-5.08270	-0.79160
H	12.86780	-4.63340	-0.18120
H	12.45270	-3.67710	-1.61380
H	14.59010	-7.39970	-3.51150
H	13.21590	-8.20730	-2.71540
H	12.94090	-7.22020	-4.16420
H	14.16950	-5.51960	-2.23580
H	7.96100	-4.48930	-0.76390

117.	GGAm_trans_WP_Conf_8		
N	8.01250	-4.37280	0.19130
C	8.91160	-3.32840	0.68690
C	10.38930	-3.36420	0.28570
N	10.80040	-4.36710	-0.51130
C	12.18610	-4.51750	-0.91690
C	13.08280	-5.03700	0.21850
N	14.36330	-4.63500	0.16830
C	15.36440	-5.11230	1.12040
O	12.64980	-5.81260	1.09280
O	11.16260	-2.47140	0.69420
H	8.29120	-5.30380	0.50580
H	8.89580	-3.32120	1.78420
H	8.53760	-2.34490	0.37540
H	10.14040	-5.08790	-0.78180
H	12.57110	-3.56540	-1.29780
H	12.22220	-5.24940	-1.73160
H	15.40880	-6.20640	1.11720
H	16.33810	-4.71320	0.83220
H	15.12830	-4.78180	2.13810
H	14.64750	-3.97240	-0.54760
H	7.96470	-4.38540	-0.82900

118.	GGAm_trans_WP_Conf_9		
N	8.05860	-4.48000	0.35720
C	8.93310	-3.37790	0.76270
C	10.39410	-3.37630	0.30310
N	10.80450	-4.37700	-0.49610
C	12.15410	-4.44360	-1.02580
C	12.39740	-3.42390	-2.15030
N	13.65630	-2.96700	-2.25020
C	14.07240	-2.06630	-3.32340
O	11.49000	-3.08710	-2.93590
O	11.15850	-2.46090	0.67890
H	7.94380	-4.52770	-0.65660
H	8.95860	-3.31190	1.85790
H	8.50690	-2.42750	0.41630
H	10.13570	-5.07640	-0.79920
H	12.30340	-5.44510	-1.44440
H	12.88240	-4.30130	-0.21990
H	15.14600	-1.89230	-3.23640
H	13.85720	-2.50740	-4.30220
H	13.54670	-1.10740	-3.25560
H	14.34470	-3.25520	-1.56050
H	8.40410	-5.38570	0.67940

119. GGA_m_trans_WP_Conf_10

N	8.20450	-4.63190	0.48590
C	8.92360	-3.36960	0.71410
C	10.39550	-3.37890	0.29630
N	10.80770	-4.37450	-0.49900
C	12.17500	-4.49440	-0.97590
C	12.28790	-5.64850	-1.97400
N	13.51280	-5.84150	-2.48940
C	13.79900	-6.90170	-3.45690
O	11.30240	-6.35030	-2.27720
O	11.15660	-2.46240	0.68240
H	8.39590	-5.29070	1.24390
H	8.90870	-3.03050	1.75860
H	8.44890	-2.57600	0.12290
H	10.13290	-5.07480	-0.79290
H	12.86440	-4.67730	-0.14010
H	12.49440	-3.56500	-1.46380
H	14.83790	-6.80640	-3.77700
H	13.65010	-7.89290	-3.01400
H	13.14610	-6.81390	-4.33140
H	14.27770	-5.24600	-2.18200
H	7.19810	-4.45770	0.52060

120. GGA_m_trans_WP_Conf_11

N	8.19670	-4.61860	0.48160
C	8.92320	-3.35900	0.70770
C	10.39460	-3.37720	0.29360
N	10.81240	-4.37550	-0.50420
C	12.19390	-4.49460	-0.94600
C	13.12250	-5.04480	0.15130
N	14.35410	-4.50800	0.20110
C	15.36430	-4.97920	1.14820
O	12.75490	-5.95840	0.91450
O	11.15480	-2.46490	0.68460
H	7.19270	-4.44830	0.57600
H	8.91080	-3.01790	1.75190
H	8.45180	-2.56350	0.11590
H	10.13090	-5.07300	-0.78730
H	12.55870	-3.52550	-1.30250
H	12.22380	-5.19840	-1.78560
H	16.24970	-4.34750	1.05970
H	14.98610	-4.92420	2.17440
H	15.64280	-6.01870	0.94180
H	14.59380	-3.74700	-0.42810
H	8.43150	-5.29400	1.21260

121.	GGAm_trans_WP_Conf_12		
N	8.04920	-4.29340	0.00070
C	8.93010	-3.37110	0.73450
C	10.39210	-3.37270	0.28840
N	10.81010	-4.37150	-0.50870
C	12.18430	-4.46680	-0.97880
C	12.50690	-3.44630	-2.08450
N	13.73040	-2.89250	-2.03250
C	14.20180	-1.95230	-3.04910
O	11.68800	-3.18990	-2.98910
O	11.15720	-2.46880	0.68930
H	7.77370	-3.88160	-0.89370
H	8.94090	-3.65520	1.79470
H	8.60650	-2.32170	0.69780
H	10.13340	-5.07760	-0.78220
H	12.32980	-5.46740	-1.40180
H	12.87840	-4.34920	-0.13940
H	15.18610	-1.58380	-2.75520
H	14.27860	-2.43770	-4.02840
H	13.51460	-1.10470	-3.14000
H	14.34680	-3.11750	-1.25650
H	7.18080	-4.41880	0.52610

122. GGA_m_trans_WP_Conf_13

N	8.00640	-4.05610	-0.19920
C	8.92460	-3.36940	0.72440
C	10.38930	-3.36960	0.28680
N	10.80830	-4.36890	-0.51040
C	12.17670	-4.44720	-1.00190
C	13.20140	-4.75330	0.10350
N	14.37450	-4.10640	0.00250
C	15.48060	-4.33550	0.93110
O	12.96200	-5.58450	1.00250
O	11.15910	-2.47220	0.69040
H	7.85820	-3.47900	-1.03090
H	8.89390	-3.87790	1.69710
H	8.66820	-2.31840	0.91030
H	10.13600	-5.07990	-0.78000
H	12.44550	-3.51780	-1.51750
H	12.22530	-5.26420	-1.73090
H	15.87390	-5.35390	0.83490
H	16.27680	-3.62370	0.70640
H	15.15270	-4.18970	1.96550
H	14.50070	-3.42380	-0.73900
H	7.08780	-4.13560	0.24380

123. GGA_m_trans_WP_Conf_14

N	8.28930	-4.69760	0.76860
C	8.92540	-3.37090	0.72840
C	10.39330	-3.37920	0.30140
N	10.81160	-4.37720	-0.49790
C	12.19130	-4.48130	-0.94970
C	12.59200	-3.37610	-1.94210
N	13.83960	-2.89690	-1.80220
C	14.40160	-1.89550	-2.70790
O	11.81780	-2.99370	-2.84200
O	11.15570	-2.46360	0.67770
H	8.62590	-5.21640	1.58330
H	8.89560	-2.83140	1.68380
H	8.39490	-2.74650	-0.00270
H	10.13210	-5.07050	-0.79440
H	12.30570	-5.44280	-1.46350
H	12.86970	-4.47690	-0.08850
H	15.40280	-1.63510	-2.36030
H	14.46750	-2.28260	-3.73080
H	13.78230	-0.99230	-2.72120
H	14.41350	-3.22620	-1.03160
H	7.28420	-4.57950	0.91620

124. GGA_m_trans_WP_Conf_15

N	8.77040	-3.12350	2.20130
C	8.92830	-3.38100	0.75980
C	10.38810	-3.36600	0.30440
N	10.80150	-4.37330	-0.49940
C	12.19300	-4.45990	-0.92660
C	13.17260	-4.76020	0.22090
N	12.73790	-5.57990	1.19040
C	13.52960	-5.89480	2.37790
O	14.31870	-4.26550	0.21050
O	11.16310	-2.46660	0.68030
H	9.27300	-2.26910	2.45330
H	8.40530	-2.59740	0.19640
H	8.45210	-4.33300	0.50440
H	10.14010	-5.08470	-0.79850
H	12.51710	-3.51690	-1.37670
H	12.27700	-5.24800	-1.68190
H	13.04740	-6.71930	2.90610
H	14.54440	-6.19100	2.09800
H	13.59210	-5.02990	3.04960
H	11.81020	-5.98500	1.11100
H	9.20950	-3.87140	2.74350

125. GGA_m_trans_WP_Conf_16

N	8.29260	-2.00240	0.51090
C	8.90790	-3.32910	0.68890
C	10.38540	-3.36020	0.29620
N	10.79890	-4.36820	-0.50630
C	12.18240	-4.43100	-0.96280
C	12.56230	-3.29840	-1.93220
N	11.61020	-2.87980	-2.78010
C	11.80040	-1.75830	-3.69820
O	13.71790	-2.82620	-1.91910
O	11.16560	-2.47160	0.68750
H	8.28520	-1.74700	-0.47940
H	8.33890	-4.07410	0.12380
H	8.84810	-3.61170	1.74770
H	10.14290	-5.09060	-0.79060
H	12.34340	-5.39370	-1.45880
H	12.87100	-4.36140	-0.11550
H	11.81760	-0.80480	-3.15620
H	12.74110	-1.86320	-4.24560
H	10.97110	-1.74750	-4.40750
H	10.70530	-3.34020	-2.76650
H	8.86600	-1.29350	0.97450

126. GGA_m_trans_WP_Conf_17

N	8.56740	-2.49800	1.79920
C	8.89110	-3.32590	0.63420
C	10.38310	-3.35390	0.28250
N	10.79910	-4.36170	-0.51780
C	12.21500	-4.53650	-0.82360
C	13.01690	-4.86400	0.44730
N	14.13090	-4.14520	0.65670
C	14.94220	-4.31160	1.86170
O	12.63680	-5.76210	1.22660
O	11.16600	-2.48050	0.69760
H	8.99850	-1.57740	1.68940
H	8.35520	-2.95140	-0.24840
H	8.53610	-4.34930	0.79910
H	10.14450	-5.09450	-0.77560
H	12.61180	-3.63970	-1.31110
H	12.31410	-5.37630	-1.51890
H	15.39790	-5.30670	1.89550
H	15.73010	-3.55690	1.85910
H	14.32800	-4.18540	2.76020
H	14.35770	-3.38590	0.02110
H	9.00610	-2.89750	2.63260

127. GGA_m_trans_WP_Conf_18

N	8.18180	-2.22890	0.11810
C	8.91950	-3.36040	0.71430
C	10.39190	-3.37420	0.30860
N	10.80510	-4.37800	-0.49410
C	12.14310	-4.37780	-1.07020
C	12.31430	-3.23780	-2.08870
N	13.47890	-2.57050	-2.04400
C	13.77060	-1.46730	-2.95810
O	11.41870	-2.97700	-2.91630
O	11.15970	-2.46100	0.67550
H	8.18330	-2.30260	-0.90210
H	8.42730	-4.29840	0.43920
H	8.88140	-3.27480	1.80620
H	10.13600	-5.07750	-0.80330
H	12.29020	-5.32760	-1.59460
H	12.89710	-4.30310	-0.27920
H	13.01940	-0.67560	-2.86150
H	14.75250	-1.05940	-2.71370
H	13.77220	-1.81100	-3.99780
H	14.15620	-2.79850	-1.32200
H	8.65230	-1.34790	0.33910

128. GGA_m_trans_WP_Conf_19

N	8.77960	-3.57320	2.18610
C	8.92430	-3.37100	0.73120
C	10.38630	-3.35980	0.28780
N	10.80000	-4.36610	-0.51220
C	12.21090	-4.53880	-0.83660
C	13.02230	-4.94460	0.40520
N	14.19910	-4.32170	0.57860
C	15.06340	-4.61010	1.72240
O	12.60150	-5.82200	1.18530
O	11.16470	-2.47330	0.69390
H	9.33290	-2.87810	2.69260
H	8.49240	-2.40050	0.46160
H	8.35830	-4.14320	0.20070
H	10.14180	-5.09150	-0.78280
H	12.61290	-3.62130	-1.27900
H	12.29580	-5.34230	-1.57560
H	15.95460	-3.98460	1.65460
H	14.54580	-4.39590	2.66410
H	15.36240	-5.66320	1.72840
H	14.47010	-3.58340	-0.06430
H	9.15420	-4.48560	2.45710

129. GGA_m_trans_WP_Conf_20

N	8.82970	-3.80140	2.18680
C	8.93830	-3.40940	0.76610
C	10.39060	-3.36450	0.29270
N	10.80350	-4.37180	-0.50880
C	12.21500	-4.57650	-0.82390
C	12.94580	-5.21570	0.36840
N	13.99140	-4.53930	0.86850
C	14.72790	-5.00700	2.04160
O	12.55600	-6.30400	0.84030
O	11.16120	-2.46760	0.69050
H	9.40370	-3.18650	2.76870
H	8.51670	-2.40650	0.64030
H	8.34650	-4.10030	0.15720
H	10.13750	-5.08670	-0.78770
H	12.67250	-3.62340	-1.10440
H	12.28070	-5.26110	-1.67460
H	15.49440	-4.27120	2.28940
H	14.05330	-5.12410	2.89700
H	15.20460	-5.97310	1.84560
H	14.25530	-3.65200	0.45110
H	9.19460	-4.74650	2.32610

130. GGA_m_trans_WP_Conf_21

N	8.16430	-2.36550	-0.19020
C	8.90490	-3.33760	0.64210
C	10.39350	-3.36790	0.29720
N	10.80580	-4.37580	-0.50550
C	12.12660	-4.38530	-1.13470
C	12.10020	-3.52290	-2.40680
N	12.74870	-2.34920	-2.35340
C	12.70200	-1.37980	-3.44690
O	11.45630	-3.89540	-3.41110
O	11.15880	-2.46350	0.68730
H	8.21200	-2.62760	-1.17790
H	8.45440	-4.32800	0.52210
H	8.81200	-3.05100	1.69440
H	10.13460	-5.08350	-0.79220
H	12.37010	-5.41340	-1.41500
H	12.87220	-4.02370	-0.42140
H	13.15670	-1.78880	-4.35520
H	11.66560	-1.10620	-3.67380
H	13.24890	-0.48610	-3.14230
H	13.26020	-2.10370	-1.51150
H	8.58780	-1.43720	-0.11650

131.	GGAm_cis_WP_Conf_1		
N	7.43980	-5.09090	0.21080
C	7.33540	-6.49090	0.62760
C	8.17030	-7.46950	-0.21680
N	8.25730	-8.76260	0.18990
C	7.61540	-9.36910	1.34950
C	8.42360	-9.38260	2.65560
N	9.67310	-8.90530	2.63030
C	10.52910	-8.86240	3.81460
O	7.87910	-9.83430	3.68670
O	8.75180	-7.09130	-1.25080
H	7.16350	-5.00170	-0.76930
H	7.63120	-6.57250	1.68040
H	6.28290	-6.80310	0.57790
H	8.78930	-9.37550	-0.42660
H	7.37920	-10.41240	1.10910
H	6.66260	-8.87820	1.57180
H	10.86120	-9.86730	4.09970
H	11.40210	-8.24800	3.58700
H	9.98920	-8.42120	4.65760
H	10.06150	-8.59560	1.74520
H	8.41720	-4.79130	0.24470

132.	GGAm_cis_WP_Conf_2		
N	7.25310	-5.13860	0.09710
C	7.42320	-6.46910	0.68400
C	8.18540	-7.46600	-0.20740
N	8.24130	-8.76660	0.17950
C	7.68420	-9.35000	1.39380
C	6.25810	-9.91300	1.29610
N	5.66280	-9.91290	0.09730
C	4.30600	-10.41230	-0.11940
O	5.71590	-10.34080	2.33800
O	8.74330	-7.09270	-1.25620
H	8.16640	-4.74740	-0.14310
H	6.43610	-6.87730	0.93180
H	7.96520	-6.37710	1.63590
H	8.79860	-9.37370	-0.42010
H	7.68230	-8.62410	2.21310
H	8.33260	-10.17540	1.70990
H	4.28680	-11.50740	-0.16770
H	3.65410	-10.08820	0.69600
H	3.93240	-10.00560	-1.06110
H	6.19390	-9.60190	-0.71000
H	6.74940	-5.21340	-0.78990

133.	GGAm_cis_WP_Conf_3		
N	7.36560	-5.11730	0.19800
C	7.37260	-6.50430	0.66710
C	8.17710	-7.47060	-0.21160
N	8.25320	-8.75870	0.17840
C	7.65890	-9.37710	1.35540
C	8.03930	-10.86540	1.36780
N	7.58430	-11.58350	2.40460
C	7.88210	-13.01150	2.52850
O	8.73370	-11.35810	0.45760
O	8.74610	-7.08270	-1.25440
H	6.99550	-5.08040	-0.75460
H	7.77580	-6.54130	1.68810
H	6.33970	-6.87180	0.73630
H	8.79210	-9.38700	-0.41660
H	6.56370	-9.29380	1.34790
H	8.02190	-8.91450	2.28310
H	7.42480	-13.38690	3.44490
H	7.48380	-13.56740	1.67280
H	8.96360	-13.17930	2.57070
H	7.01890	-11.13370	3.12120
H	8.32750	-4.77780	0.12390

134.	GGAm_cis_WP_Conf_4		
N	7.32950	-5.14820	0.08320
C	7.26590	-6.52910	0.58310
C	8.16240	-7.47120	-0.22340
N	8.26630	-8.76160	0.19650
C	7.58040	-9.36960	1.32990
C	8.38940	-9.52660	2.62680
N	9.71380	-9.34220	2.57260
C	10.58320	-9.50550	3.73720
O	7.78300	-9.85430	3.67010
O	8.75620	-7.08810	-1.24800
H	6.63970	-4.59440	0.59670
H	6.24560	-6.94430	0.55620
H	7.58150	-6.53860	1.63410
H	8.78370	-9.37810	-0.42930
H	7.24720	-10.37500	1.04300
H	6.68000	-8.80610	1.58650
H	10.49900	-8.65210	4.42020
H	10.31530	-10.41430	4.28330
H	11.61550	-9.58570	3.39200
H	10.13350	-9.06580	1.69040
H	7.03080	-5.12290	-0.89420

135. GGAm_cis_WP_Conf_5

N	7.46850	-5.11440	0.15950
C	7.49320	-6.47070	0.72680
C	8.19290	-7.46360	-0.20370
N	8.23330	-8.76980	0.17550
C	7.69110	-9.34300	1.40110
C	6.34720	-10.07800	1.28570
N	5.89740	-10.38900	0.06390
C	4.65600	-11.13030	-0.15630
O	5.74900	-10.39010	2.33840
O	8.73920	-7.09290	-1.25890
H	8.42460	-4.80670	-0.03150
H	8.00590	-6.51420	1.70090
H	6.46070	-6.80110	0.89970
H	8.80320	-9.37270	-0.41720
H	7.56370	-8.57290	2.16540
H	8.41100	-10.06680	1.80430
H	3.77800	-10.48880	-0.01740
H	4.65800	-11.51680	-1.17710
H	4.58860	-11.96690	0.54470
H	6.42970	-10.08700	-0.74610
H	7.11290	-4.47730	0.87650

136.	GGAm_cis_WP_Conf_6		
N	7.31170	-5.15330	0.05910
C	7.27320	-6.52490	0.58640
C	8.16430	-7.47070	-0.22180
N	8.26380	-8.76210	0.19550
C	7.59680	-9.36650	1.34200
C	8.45540	-9.61300	2.59060
N	9.78290	-9.47680	2.48660
C	10.69120	-9.73420	3.60350
O	7.88210	-9.96840	3.64330
O	8.75530	-7.08950	-1.24880
H	7.03780	-5.15730	-0.92590
H	7.61120	-6.51310	1.63080
H	6.25700	-6.95020	0.58820
H	8.78530	-9.37660	-0.42930
H	7.18730	-10.34120	1.04600
H	6.74780	-8.75680	1.65910
H	10.41660	-10.66670	4.10460
H	11.70650	-9.82250	3.21280
H	10.65910	-8.92220	4.33920
H	10.17810	-9.16400	1.60540
H	6.59410	-4.60750	0.54230

137. GGA_m_cis_WP_Conf_7

N	7.34130	-5.10910	0.10600
C	7.35650	-6.47630	0.63360
C	8.17610	-7.47030	-0.20860
N	8.24810	-8.76280	0.18630
C	7.67880	-9.38590	1.37630
C	8.76780	-9.77180	2.39190
N	8.78940	-11.06150	2.76570
C	9.75050	-11.57320	3.74170
O	9.56400	-8.92210	2.83730
O	8.74990	-7.10040	-1.25360
H	8.29850	-4.75550	0.03710
H	7.75270	-6.46110	1.65610
H	6.32370	-6.84240	0.70520
H	8.79470	-9.36540	-0.42840
H	7.09500	-10.26500	1.08020
H	6.99770	-8.69210	1.87630
H	9.55940	-11.16030	4.73880
H	9.66240	-12.66010	3.78160
H	10.77100	-11.30580	3.44940
H	8.12190	-11.70870	2.35610
H	6.98740	-5.11540	-0.85340

138. GGA_m_cis_WP_Conf_8

N	7.41330	-5.09130	0.15190
C	7.39630	-6.46590	0.65970
C	8.17560	-7.47070	-0.20890
N	8.24860	-8.76260	0.18660
C	7.62730	-9.39710	1.34380
C	6.53870	-10.39740	0.91910
N	6.67230	-11.64500	1.39770
C	5.70860	-12.70310	1.09620
O	5.59520	-10.04890	0.18220
O	8.75010	-7.10020	-1.25340
H	7.05530	-5.07330	-0.80580
H	7.81620	-6.47650	1.67410
H	6.35610	-6.80190	0.75030
H	8.79430	-9.36550	-0.42860
H	7.14940	-8.64350	1.97470
H	8.39640	-9.89400	1.94640
H	5.55810	-12.78490	0.01510
H	6.09870	-13.64880	1.47610
H	4.73850	-12.50000	1.56390
H	7.46940	-11.86790	1.98690
H	8.37920	-4.76240	0.08390

139. GGAm_cis_WP_Conf_9

N	7.13660	-5.21560	0.03610
C	7.41730	-6.49880	0.69770
C	8.18630	-7.46470	-0.20910
N	8.24240	-8.76730	0.17790
C	7.63410	-9.34170	1.37450
C	6.11230	-9.55890	1.31440
N	5.54050	-9.63200	0.10490
C	4.09530	-9.76390	-0.07590
O	5.47090	-9.65740	2.38160
O	8.74190	-7.08670	-1.25670
H	6.53300	-5.37300	-0.77520
H	8.04000	-6.31540	1.58610
H	6.50510	-6.99060	1.05940
H	8.79800	-9.38030	-0.41640
H	7.82850	-8.72170	2.25580
H	8.10410	-10.31480	1.56070
H	3.71950	-10.67600	0.39890
H	3.57340	-8.90490	0.36070
H	3.88470	-9.80160	-1.14600
H	6.13040	-9.59650	-0.72080
H	6.58100	-4.64520	0.67820

140.	GGAm_cis_WP_Conf_10		
N	7.55260	-5.10910	0.29940
C	7.32780	-6.52200	0.64030
C	8.16990	-7.46900	-0.21980
N	8.26010	-8.76290	0.18930
C	7.62940	-9.34110	1.37210
C	8.29140	-8.99930	2.71820
N	9.57310	-8.60960	2.70090
C	10.28450	-8.18660	3.90680
O	7.61950	-9.09540	3.76680
O	8.75110	-7.08410	-1.25080
H	8.53040	-4.86550	0.47750
H	7.51890	-6.73100	1.70080
H	6.27020	-6.76880	0.46380
H	8.78750	-9.38300	-0.42300
H	7.63630	-10.43200	1.26220
H	6.58060	-9.03670	1.45180
H	10.29130	-8.98130	4.65950
H	11.31160	-7.94150	3.63180
H	9.81030	-7.29970	4.34260
H	10.07200	-8.59970	1.81640
H	7.00920	-4.53880	0.95220

141.	GGAm_cis_WP_Conf_11		
N	7.35900	-5.14320	0.13530
C	7.30590	-6.52990	0.61830
C	8.17040	-7.47200	-0.21920
N	8.25910	-8.76280	0.19040
C	7.64010	-9.35000	1.37490
C	6.10330	-9.42840	1.29470
N	5.44890	-9.21120	2.44850
C	3.98810	-9.23850	2.53330
O	5.52100	-9.69520	0.22600
O	8.75170	-7.08500	-1.25150
H	7.03370	-5.10660	-0.83370
H	6.28350	-6.93510	0.61430
H	7.65150	-6.55830	1.66020
H	8.78730	-9.37920	-0.42400
H	7.94790	-8.81720	2.28290
H	8.01340	-10.37750	1.46180
H	3.69650	-9.08030	3.57290
H	3.54900	-8.44700	1.91510
H	3.59340	-10.20020	2.19090
H	5.97610	-8.97440	3.28450
H	6.67960	-4.59880	0.67240

142. GGA_m_cis_WP_Conf_12

N	7.40240	-5.13000	0.15200
C	7.36510	-6.50910	0.65760
C	8.17160	-7.47100	-0.21700
N	8.25670	-8.76310	0.18960
C	7.62480	-9.36530	1.35930
C	6.19400	-9.86610	1.09130
N	5.30530	-9.66460	2.07950
C	3.93020	-10.16040	2.01070
O	5.90730	-10.45110	0.02850
O	8.75130	-7.08890	-1.25180
H	6.90010	-4.53790	0.81800
H	7.73760	-6.59450	1.68970
H	6.32070	-6.84820	0.67360
H	8.78900	-9.37600	-0.42510
H	7.64450	-8.67330	2.20650
H	8.22070	-10.23960	1.64940
H	3.34820	-9.68950	2.80460
H	3.48570	-9.90940	1.04370
H	3.89280	-11.24890	2.13520
H	5.59970	-9.18310	2.92430
H	8.36670	-4.78920	0.15370

143. GGA_m_cis_WP_Conf_13

N	7.36410	-5.13950	0.12950
C	7.37860	-6.50660	0.66700
C	8.18390	-7.46800	-0.20940
N	8.24380	-8.76640	0.18090
C	7.66580	-9.35340	1.38560
C	8.59460	-9.27050	2.61050
N	7.99730	-9.00190	3.78420
C	8.72970	-8.96870	5.05070
O	9.81980	-9.47340	2.50160
O	8.74430	-7.08970	-1.25620
H	6.93020	-5.13620	-0.79640
H	7.83240	-6.48430	1.66670
H	6.36930	-6.92840	0.78900
H	8.79660	-9.37480	-0.41970
H	7.48840	-10.41780	1.18880
H	6.69180	-8.90490	1.60320
H	9.64990	-8.38860	4.93910
H	8.09940	-8.49760	5.80700
H	8.99550	-9.97870	5.38370
H	6.99280	-8.85100	3.80810
H	6.75380	-4.57320	0.72340

144. GGAm_cis_WP_Conf_14

N	7.38250	-5.13840	0.14090
C	7.45730	-6.49050	0.71230
C	8.18730	-7.46780	-0.20820
N	8.24110	-8.76700	0.17850
C	7.62790	-9.35310	1.36660
C	8.27980	-8.89510	2.68580
N	7.43940	-8.72800	3.72160
C	7.90300	-8.29180	5.03930
O	9.50930	-8.71520	2.77530
O	8.74230	-7.08750	-1.25760
H	8.32730	-4.79570	-0.04770
H	7.97750	-6.50810	1.68170
H	6.43870	-6.85700	0.89530
H	8.79800	-9.37660	-0.41710
H	7.75820	-10.43990	1.29900
H	6.54860	-9.15930	1.38610
H	8.32550	-7.28180	4.98820
H	7.05330	-8.28690	5.72380
H	8.67290	-8.96710	5.42560
H	6.44160	-8.86050	3.58110
H	7.00110	-4.51580	0.85750

145. GGAm_cis_WP_Conf_15

N	8.26350	-6.03260	1.80230
C	7.42810	-6.44790	0.65480
C	8.17990	-7.47020	-0.20570
N	8.24370	-8.76390	0.18400
C	7.66270	-9.40010	1.36640
C	8.67560	-9.65300	2.50390
N	9.26570	-8.56660	3.01280
C	10.25340	-8.63290	4.08590
O	8.89560	-10.81750	2.90790
O	8.74800	-7.09890	-1.25630
H	9.01460	-5.41710	1.48480
H	6.49320	-6.86860	1.03840
H	7.16680	-5.61940	-0.01350
H	8.79710	-9.36600	-0.42640
H	7.25500	-10.37060	1.07380
H	6.83800	-8.79360	1.75100
H	11.09770	-9.26960	3.80150
H	10.62160	-7.62270	4.27830
H	9.81360	-9.03220	5.00670
H	8.98140	-7.64000	2.65180
H	7.69960	-5.47350	2.44360

146. GGA_m_cis_WP_Conf_16

N	5.89840	-6.64390	0.30380
C	7.33790	-6.47160	0.59780
C	8.17000	-7.47260	-0.21230
N	8.25430	-8.76130	0.19090
C	7.65610	-9.40200	1.36220
C	6.39580	-10.23570	1.04640
N	5.35640	-9.55790	0.54860
C	4.09670	-10.19980	0.18390
O	6.37880	-11.46660	1.27220
O	8.75340	-7.09740	-1.25260
H	5.68490	-6.27750	-0.62570
H	7.49480	-6.61020	1.67240
H	7.71640	-5.47720	0.33560
H	8.79080	-9.36760	-0.43040
H	7.40710	-8.64890	2.11490
H	8.39190	-10.08070	1.80050
H	3.43720	-9.44420	-0.24890
H	4.25950	-10.99260	-0.55390
H	3.60580	-10.63830	1.06010
H	5.45130	-8.53440	0.43150
H	5.35210	-6.07940	0.95560

147. GGA_m_cis_WP_Conf_17

N	7.95040	-5.15720	0.70710
C	7.34230	-6.49980	0.62940
C	8.18000	-7.46950	-0.21050
N	8.24690	-8.76500	0.18410
C	7.76430	-9.33370	1.44100
C	8.52030	-8.79050	2.66920
N	7.78790	-8.63090	3.78560
C	8.37020	-8.12110	5.02670
O	9.73460	-8.52000	2.61180
O	8.74690	-7.09170	-1.25510
H	7.35240	-4.57930	1.30350
H	6.37180	-6.42200	0.11930
H	7.13390	-6.92040	1.61730
H	8.79480	-9.37270	-0.42280
H	7.93840	-10.41520	1.39710
H	6.68470	-9.18690	1.55580
H	7.56470	-7.93140	5.73790
H	9.07510	-8.83830	5.46150
H	8.90580	-7.18580	4.83560
H	6.80280	-8.88240	3.78120
H	8.84530	-5.21090	1.20220

148. GGA_m_cis_WP_Conf_18

N	6.57310	-5.55370	-0.11210
C	7.41470	-6.47880	0.67420
C	8.17500	-7.47090	-0.21340
N	8.25200	-8.76360	0.18750
C	7.52740	-9.39740	1.28960
C	6.00510	-9.42750	1.05480
N	5.23630	-9.22500	2.13890
C	3.77540	-9.21450	2.06050
O	5.53450	-9.62090	-0.08210
O	8.74980	-7.09120	-1.25350
H	5.81360	-6.07190	-0.56290
H	8.18620	-5.89620	1.19540
H	6.84870	-7.00070	1.45030
H	8.79180	-9.37320	-0.42500
H	7.76460	-8.92280	2.24790
H	7.87430	-10.43550	1.34910
H	3.37610	-10.21590	1.86440
H	3.37740	-8.84760	3.00790
H	3.44820	-8.55090	1.25420
H	5.67160	-9.10100	3.04960
H	6.10850	-4.92170	0.54530