

XYZ coordinates

for Table S6

38

3a''-2H2O G -825.798540

C	1.0789150	0.4699830	0.7586130
C	-0.2731660	-0.1703570	0.5616240
C	-0.3741280	-1.6493140	0.8804610
C	0.9441340	-2.2253690	1.4194930
C	2.1032330	-1.7897760	0.5585420
C	2.1636740	-0.4307940	0.2166910
H	-1.1948580	-1.8102770	1.5874610
H	1.1111090	1.4601060	0.3000080
H	1.2214870	0.5973650	1.8432480
H	-0.6576410	-2.1680510	-0.0440070
N	-1.2388910	0.5404110	0.1202710
O	2.0535940	3.2015220	-1.2339450
H	1.0786790	3.2324980	-1.1634560
H	2.3646670	4.0758150	-0.9776600
O	-0.7031540	3.0852860	-0.8912010
H	-1.2576220	3.2208040	-1.6674210
H	-0.9524380	2.2024770	-0.5203300
C	-2.5188280	-0.0439500	-0.0761890
C	-3.4498230	-0.0686670	0.9663390
C	-2.8740310	-0.5249580	-1.3397350
C	-4.7228210	-0.5920580	0.7473280
H	-3.1685180	0.3233270	1.9394470
C	-4.1489350	-1.0478580	-1.5499600
H	-2.1465780	-0.4874340	-2.1455500
C	-5.0771680	-1.0845550	-0.5091120
H	-5.4403520	-0.6115950	1.5617800
H	-4.4170430	-1.4248470	-2.5320640
H	-6.0699420	-1.4889080	-0.6769650
C	3.1866670	0.0465830	-0.6018080
C	3.0830720	-2.6605270	0.0825790
C	4.1180210	-2.1820310	-0.7231700
H	4.8781230	-2.8653910	-1.0891510
C	4.1679260	-0.8312010	-1.0668520
H	4.9662080	-0.4616580	-1.7031080
H	3.1975350	1.0995070	-0.8747120
H	3.0354690	-3.7155380	0.3406350
H	1.0978310	-1.8680350	2.4466190
H	0.8824930	-3.3154570	1.4680900

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3a'-2H2O TS G -825.752632 -ifreq = -900.67

C	-1.1342360	0.8244080	-0.3218690
C	0.0480050	0.0022660	-0.1461400
C	-0.1119870	-1.4048000	0.3508210
C	-1.3067450	-2.0738340	-0.3382250
C	-2.5639090	-1.2551440	-0.1762420
C	-2.4604960	0.1439820	-0.1873580
H	0.8049540	-1.9780560	0.2032190
H	-0.9812050	1.7344300	0.5105710
H	-1.0617710	1.4494950	-1.2194300
H	-0.3012220	-1.3517660	1.4320270
N	1.2235060	0.5351070	-0.3674250
O	-0.6128900	2.9840330	1.1134150
H	0.4247610	3.1926350	0.2203040
H	-0.3376860	2.9277000	2.0357650
O	1.1928740	3.1563290	-0.5368860
H	0.9320130	3.7194270	-1.2729350
H	1.2407360	1.5681380	-0.6400260
C	2.4997530	-0.0585370	-0.1289990
C	3.4433920	-0.0164260	-1.1555370
C	2.8277530	-0.5963200	1.1161370
C	4.7152510	-0.5427140	-0.9417390
H	3.1738000	0.4226560	-2.1109950
C	4.0996220	-1.1277630	1.3188660

H	2.0999180	-0.5820200	1.9212570
C	5.0433790	-1.1043830	0.2921790
H	5.4485640	-0.5139000	-1.7408160
H	4.3551290	-1.5487130	2.2856700
H	6.0343150	-1.5145570	0.4563920
C	-3.6226500	0.9146190	-0.0664830
C	-3.8175980	-1.8558250	-0.0406490
C	-4.9711360	-1.0821200	0.0715760
H	-5.9395960	-1.5611560	0.1755050
C	-4.8711340	0.3098560	0.0552990
H	-5.7626540	0.9225070	0.1468200
H	-3.5379520	1.9985550	-0.0650160
H	-3.8877150	-2.9408780	-0.0272340
H	-1.0798760	-2.1984820	-1.4052900
H	-1.4461960	-3.0760710	0.0753060

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3a'-2H2O G -825.794467

C	-1.1538070	0.5641440	-0.4366840
C	-0.0540440	-0.2276960	-0.4474340
C	-0.1939790	-1.6982430	-0.1068140
C	-1.5128330	-2.2349690	-0.6652520
C	-2.6796750	-1.3803380	-0.2284900
C	-2.4810700	0.0139090	-0.1511180
H	0.6547780	-2.2588070	-0.5076650
H	0.1719890	1.5329930	1.4349040
H	-1.0658600	1.6240780	-0.6713680
H	-0.1935640	-1.8337170	0.9825870
N	1.1769630	0.2658310	-0.8635000
O	0.9019260	2.1344650	1.6509720
H	1.0999100	3.0471820	0.0171330
H	1.6748430	1.5612890	1.7542630
O	1.0601910	3.1816090	-0.9483730
H	1.5823050	3.9657590	-1.1469360
H	1.1398680	1.1950500	-1.2798890
C	2.4214020	-0.0373340	-0.3000480
C	3.5714010	0.4147230	-0.9709630
C	2.5751580	-0.7221720	0.9151400
C	4.8350670	0.1730270	-0.4484210
H	3.4552490	0.9526850	-1.9076140
C	3.8522120	-0.9765530	1.4200680
H	1.7071190	-1.0482510	1.4767500
C	4.9878580	-0.5347390	0.7475340
H	5.7088510	0.5328100	-0.9830070
H	3.9492070	-1.5136390	2.3586510
H	5.9764170	-0.7298750	1.1489680
C	-3.5613510	0.8400160	0.1847490
C	-3.9378750	-1.9122240	0.0412210
C	-5.0085130	-1.0822320	0.3836110
H	-5.9834220	-1.5111180	0.5927940
C	-4.8171540	0.2974240	0.4513530
H	-5.6436960	0.9508580	0.7131930
H	-3.4099000	1.9152040	0.2393300
H	-4.0845160	-2.9879350	-0.0213600
H	-1.4642720	-2.2322610	-1.7634570
H	-1.6599840	-3.2720380	-0.3504870

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3a''-3H2O G -902.190508

C	-0.9718770	0.3060290	-0.6765630
C	0.4215070	-0.2285860	-0.4460890
C	0.6078770	-1.7270530	-0.5731320
C	-0.6458320	-2.4263110	-1.1181590
C	-1.8641980	-1.9963900	-0.3405140
C	-2.0157830	-0.6223480	-0.1057730
H	1.4842290	-1.9271790	-1.1989050
H	-1.0702740	1.3137200	-0.2700550
H	-1.1089450	0.3813520	-1.7668920
H	0.8412810	-2.1220000	0.4233840
N	1.3581840	0.5957490	-0.1677890
O	-1.9615360	3.1539410	1.0336050
H	-0.9994980	3.2994210	0.9584720

H	-2.2782910	3.7374400	1.7313740
O	0.6295700	3.2317640	0.0292890
H	1.3739850	3.8128160	0.2208530
H	0.9859330	2.3026300	-0.0286010
O	-1.5762680	3.6686940	-1.7940920
H	-0.6715190	3.6051140	-1.4499460
H	-2.1140530	3.5508360	-0.9968050
C	2.6826660	0.1283640	0.0488170
C	3.6391820	0.2753290	-0.9594840
C	3.0508420	-0.4039080	1.2879160
C	4.9523490	-0.1347620	-0.7348340
H	3.3440270	0.7052040	-1.9120680
C	4.3671680	-0.8064850	1.5061640
H	2.3038700	-0.4955200	2.0712810
C	5.3214760	-0.6766570	0.4966170
H	5.6892120	-0.0256960	-1.5245190
H	4.6469840	-1.2210930	2.4696450
H	6.3455510	-0.9904430	0.6701060
C	-3.1018440	-0.1496150	0.6299940
C	-2.8126400	-2.8866850	0.1623310
C	-3.9081930	-2.4135990	0.8868910
H	-4.6433670	-3.1126290	1.2734970
C	-4.0517990	-1.0462900	1.1219390
H	-4.8986720	-0.6786680	1.6930910
H	-3.1884980	0.9181360	0.8173070
H	-2.6934370	-3.9531020	-0.0120880
H	-0.7732180	-2.1629860	-2.1767170
H	-0.5174450	-3.5106560	-1.0721740

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3a'' TS G -902.436892

C	-1.0363470	0.5017600	-0.1913560
C	0.1945490	-0.2525170	-0.1071380
C	0.1344540	-1.6920300	0.3092260
C	-1.0237820	-2.3989080	-0.4055920
C	-2.3301340	-1.6694490	-0.2048380
C	-2.3165200	-0.2693040	-0.1287720
H	1.0842300	-2.1955040	0.1215930
H	-0.9490630	1.2879610	0.7564210
H	-1.0203370	1.2485540	-0.9935410
H	-0.0442070	-1.7093850	1.3933250
N	1.3321250	0.3599570	-0.3307180
O	-0.7158620	2.5070350	1.5008490
H	0.5107980	2.9530020	0.5469660
H	-0.8134580	2.5102160	2.4583680
O	1.0397230	3.0740900	-0.3005220
H	0.3990460	3.5104060	-0.8819090
H	1.2742060	1.3820550	-0.5516900
O	-1.8013820	3.7239850	-0.5480710
H	-1.5579940	3.3774600	0.3530190
H	-2.2426550	4.5691220	-0.4171320
C	2.6490560	-0.1667280	-0.1518590
C	3.5527300	-0.0532400	-1.2076320
C	3.0410030	-0.7179140	1.0680190
C	4.8552300	-0.5204020	-1.0468320
H	3.2301800	0.3928740	-2.1431540
C	4.3430600	-1.1907260	1.2167020
H	2.3378520	-0.7603600	1.8939630
C	5.2501150	-1.0945770	0.1614820
H	5.5598380	-0.4365880	-1.8674790
H	4.6503900	-1.6227440	2.1632410
H	6.2647140	-1.4590800	0.2834330
C	-3.5243470	0.4227840	0.0166610
C	-3.5460440	-2.3527160	-0.1257340
C	-4.7462720	-1.6588420	0.0155930
H	-5.6842460	-2.2018780	0.0753080
C	-4.7335540	-0.2645770	0.0830450
H	-5.6633250	0.2848940	0.1936610
H	-3.5015680	1.5088300	0.0722670
H	-3.5495360	-3.4387520	-0.1802150
H	-0.7964840	-2.4616750	-1.4778770

H	-1.0977170	-3.4254650	-0.0373810
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3a'-3H2O G -902.186709

C	0.9421520	0.2285590	-1.0572610
C	-0.0885720	-0.2357300	-0.3178310
C	0.1795370	-1.2113430	0.8115850
C	1.4817160	-0.8339070	1.5202530
C	2.6195080	-0.6626480	0.5398860
C	2.3261940	-0.1176080	-0.7291260
H	-0.6554960	-1.2131600	1.5184520
H	-1.2081370	1.4625840	1.4200000
H	0.7578090	0.9036680	-1.8897960
H	0.2696100	-2.2298210	0.4130210
N	-1.3768290	0.2686890	-0.4800480
O	-0.9452310	2.3254730	1.7744240
H	2.2713710	2.0610350	0.5511690
H	0.0272160	2.3494280	1.7033350
O	1.6461830	2.7777230	0.7233010
H	1.1226370	2.8666530	-0.0923090
H	-1.4270500	1.1309150	-1.0180000
O	-0.7249590	3.1440270	-0.8676780
H	-1.0618450	3.1748540	0.0481410
H	-0.9847840	3.9672190	-1.2960680
C	-2.5696720	-0.4644480	-0.3680180
C	-3.7685920	0.2414140	-0.1844280
C	-2.6037320	-1.8618560	-0.4453950
C	-4.9746580	-0.4409360	-0.0750620
H	-3.7405730	1.3265300	-0.1240580
C	-3.8161370	-2.5375720	-0.3093690
H	-1.6920460	-2.4171090	-0.6365830
C	-5.0061700	-1.8367580	-0.1248090
H	-5.8937270	0.1200650	0.0630100
H	-3.8269020	-3.6216490	-0.3677080
H	-5.9469390	-2.3680790	-0.0279840
C	3.3747860	0.1186410	-1.6294440
C	3.9381310	-0.9706850	0.8675320
C	4.9748340	-0.7430410	-0.0403860
H	5.9968030	-0.9896300	0.2292240
C	4.6895130	-0.1943060	-1.2905220
H	5.4893440	-0.0099140	-2.0009650
H	3.1496560	0.5460910	-2.6032810
H	4.1574300	-1.3895930	1.8467000
H	1.3348580	0.1140140	2.0598470
H	1.7355610	-1.5894040	2.2691240

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3a'-PhOH-2H2O G -1133.076958

C	-1.7815230	-0.5690230	0.8273390
C	-1.1611510	0.7827370	0.5737600
C	-2.0995020	1.9708860	0.5569250
C	-3.5364770	1.5866240	0.9388560
C	-3.9831310	0.3793730	0.1529270
C	-3.0911000	-0.7005580	0.0866680
H	-1.7025910	2.7494980	1.2172670
H	-1.0908220	-1.3722060	0.5645670
H	-1.9665430	-0.6369670	1.9109830
H	-2.0871730	2.3895880	-0.4570550
N	0.1013120	0.8618820	0.3827010
O	-0.4408430	-3.6320970	-0.4516770
H	-0.3535110	-3.7640660	0.5065300
H	0.2044920	-2.9340820	-0.6332900
O	1.4215390	-1.4544210	0.3201500
H	1.0070310	-0.5298820	0.3293860
O	0.3094120	-3.1435710	2.2716690
H	0.8831460	-2.5040190	1.8143300
H	0.8800970	-3.6613200	2.8497200
C	0.7157210	2.1238110	0.1471940
C	1.3441230	2.7928900	1.2003990
C	0.7761880	2.6419310	-1.1490780
C	2.0118540	3.9921190	0.9572460
H	1.3069280	2.3668240	2.1986710

C	1.4485020	3.8402260	-1.3836530
H	0.3028920	2.0993900	-1.9624530
C	2.0664980	4.5194980	-0.3332590
H	2.4954140	4.5112200	1.7787830
H	1.4923010	4.2402060	-2.3917800
H	2.5918310	5.4502690	-0.5200830
C	-3.4171270	-1.8424560	-0.6441800
C	-5.2060660	0.2996560	-0.5125000
C	-5.5415040	-0.8485250	-1.2324730
H	-6.4959750	-0.9042810	-1.7467530
C	-4.6476200	-1.9169710	-1.2995210
H	-4.9043920	-2.8057310	-1.8675270
H	-2.7010020	-2.6597220	-0.6990980
H	-5.8968480	1.1379480	-0.4690850
H	-3.5745970	1.3603120	2.0128410
H	-4.2059220	2.4331810	0.7674190
C	2.7325200	-1.4479280	-0.0528100
C	3.4135710	-0.2657380	-0.3563950
C	3.3919060	-2.6778410	-0.1272710
C	4.7548070	-0.3245650	-0.7332940
H	2.8981430	0.6892140	-0.2978970
C	4.7316200	-2.7215180	-0.5040620
H	2.8425940	-3.5855760	0.1067480
C	5.4217440	-1.5469530	-0.8092910
H	5.2786390	0.5969020	-0.9687490
H	5.2375340	-3.6804440	-0.5611880
H	6.4651630	-1.5847560	-1.1034920

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3a'' PH2H2O TS G -1133.037233 ifreq = -917.69

C	-1.8362040	0.3130460	-0.4055560
C	-0.9167750	-0.7811790	-0.2470120
C	-1.4180140	-2.0671420	0.3381550
C	-2.7661800	-2.4298970	-0.2974110
C	-3.7598220	-1.3003070	-0.1729810
C	-3.2944940	0.0208300	-0.2483110
H	-0.6887320	-2.8678990	0.2061920
H	-1.4135110	1.0800540	0.4904030
H	-1.5985560	0.9620870	-1.2561220
H	-1.5555070	-1.9113910	1.4169740
N	0.3514450	-0.5990940	-0.5475290
O	-0.7091580	2.1208450	1.1491880
H	0.3983970	2.2153620	0.2523810
H	-0.5625110	2.0059260	2.0950380
O	1.0597150	2.2162310	-0.5699190
H	0.5887020	0.3182240	-0.9442420
O	-2.4414050	3.9353290	0.1839820
H	-1.7835320	3.3361910	0.6131340
H	-1.9342360	4.6691800	-0.1774570
C	1.4638490	-1.4531260	-0.2716290
C	2.4220040	-1.6204540	-1.2703210
C	1.6338500	-2.0312340	0.9862190
C	3.5517570	-2.3925860	-1.0116230
H	2.2834320	-1.1418260	-2.2350410
C	2.7590220	-2.8150030	1.2299410
H	0.9126670	-1.8435330	1.7750990
C	3.7183230	-2.9976140	0.2340770
H	4.3013140	-2.5197500	-1.7855960
H	2.8937190	-3.2659120	2.2074770
H	4.5988130	-3.5997160	0.4322120
C	-4.2051480	1.0807100	-0.1637010
C	-5.1260970	-1.5414890	-0.0129630
C	-6.0315180	-0.4848970	0.0633220
H	-7.0910900	-0.6854500	0.1873310
C	-5.5671290	0.8289500	-0.0144960
H	-6.2648080	1.6583110	0.0490200
H	-3.8340780	2.1029000	-0.2104760
H	-5.4808680	-2.5674550	0.0489350
H	-2.6085680	-2.6712060	-1.3568140
H	-3.1523630	-3.3344480	0.1794050
C	2.3343040	1.9238110	-0.2285890

C	2.6750420	1.4549780	1.0481240
C	3.3335410	2.0480330	-1.2035890
C	3.9952940	1.1115570	1.3349800
H	1.8983940	1.3462890	1.8003170
C	4.6487660	1.7032580	-0.9048430
H	3.0567510	2.4131580	-2.1880430
C	4.9906150	1.2311620	0.3645380
H	4.2438720	0.7421140	2.3258560
H	5.4127860	1.8038040	-1.6703300
H	6.0162690	0.9609610	0.5930510

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3a' PhOH2H2O G -1133.070936

C	-2.0021950	-1.0440680	0.7341760
C	-0.8031590	-0.9933920	0.1261850
C	-0.6905190	-0.4558640	-1.2855810
C	-1.6728650	0.7010010	-1.4742130
C	-3.0684280	0.3070320	-1.0502400
C	-3.2077140	-0.5431700	0.0658820
H	0.3348800	-0.1279770	-1.4859240
H	0.9701460	0.4311590	0.9813340
H	-2.0909890	-1.4411000	1.7432110
H	-0.9229950	-1.2465710	-2.0105550
N	0.3899470	-1.2805090	0.8245120
O	1.0660760	1.3950580	1.1893940
H	-0.7917090	2.1234640	1.4768820
O	-1.6734930	2.1394000	1.8776650
H	-1.7324020	1.2666870	2.2913270
H	0.2414680	-1.3857530	1.8281390
O	-0.1240650	0.0306500	3.3650080
H	0.4799950	0.7657600	3.1835230
H	-0.2476730	0.0132340	4.3209070
C	1.4032330	-2.1255430	0.3002120
C	2.6489610	-2.1279490	0.9427420
C	1.2057200	-2.9324440	-0.8227600
C	3.6820160	-2.9256690	0.4634550
H	2.7979810	-1.4940480	1.8137820
C	2.2551820	-3.7132450	-1.3096340
H	0.2336220	-2.9702080	-1.3016900
C	3.4942100	-3.7155400	-0.6733910
H	4.6408600	-2.9206500	0.9721390
H	2.0918290	-4.3338900	-2.1851110
H	4.3043380	-4.3287150	-1.0536650
C	-4.4883590	-0.8731100	0.5232790
C	-4.2075240	0.7937730	-1.6858330
C	-5.4834890	0.4529220	-1.2297440
H	-6.3619190	0.8390060	-1.7372430
C	-5.6222890	-0.3809150	-0.1212650
H	-6.6101070	-0.6477660	0.2412820
H	-4.5923510	-1.5235970	1.3880860
H	-4.0968820	1.4511060	-2.5448470
H	-1.3492430	1.5500640	-0.8549600
H	-1.6692840	1.0344870	-2.5157640
C	1.9371380	2.0069790	0.3326920
C	2.0301770	3.3989010	0.3859970
C	2.7173750	1.2798160	-0.5694550
C	2.9072070	4.0614950	-0.4687430
H	1.4146470	3.9431980	1.0955710
C	3.5895140	1.9570790	-1.4214610
H	2.6510440	0.1942560	-0.5950310
C	3.6899600	3.3470020	-1.3776490
H	2.9766850	5.1439210	-0.4244590
H	4.1945430	1.3882550	-2.1206680
H	4.3708280	3.8678240	-2.0422900

For Table S7

32

3a' rK G -672.953797

C	2.3907080	-0.6443840	0.2037370
C	3.5379330	-1.4680230	0.2986890
C	4.7843800	-0.9568190	0.0089090

H	5.6609380	-1.5886030	0.0702260
C	2.5314590	0.7236670	-0.1587140
H	3.4180770	-2.5058180	0.5869210
C	4.9121410	0.3849360	-0.3686560
H	5.8914810	0.7864320	-0.5985340
C	1.1069800	-1.1766410	0.4735560
C	-0.0664490	-0.4574410	0.1711790
C	3.7936960	1.2148730	-0.4449760
H	3.9110860	2.2557150	-0.7229900
C	1.3127600	1.6033450	-0.1388750
H	1.4568690	2.4655580	-0.7895750
C	0.0513390	0.8475230	-0.5577740
H	0.1138520	0.5834790	-1.6214040
H	-0.8330540	1.4657330	-0.4315770
H	1.1793600	1.9850770	0.8797490
H	1.0205050	-2.1770280	0.8839450
N	-1.2407650	-1.0039480	0.4430900
H	-1.2355040	-1.9470540	0.8234380
C	-2.5335210	-0.4191260	0.2442740
C	-3.4415840	-1.0746760	-0.5799590
C	-2.8740810	0.7540180	0.9112660
C	-4.7081660	-0.5296470	-0.7543810
H	-3.1525620	-1.9900400	-1.0816590
C	-4.1409180	1.2920040	0.7232340
H	-2.1606190	1.2248770	1.5772900
C	-5.0560700	0.6530170	-0.1088230
H	-5.4206730	-1.0293520	-1.3982810
H	-4.4147440	2.2047230	1.2369330
H	-6.0436340	1.0743530	-0.2489760

32

3a' N G -673.142598

C	2.3426800	-0.5995300	0.2166950
C	3.4782310	-1.3650800	0.4987690
C	4.7493180	-0.8049590	0.4269020
H	5.6199400	-1.4124810	0.6443670
C	2.4980270	0.7569040	-0.1289100
H	3.3587950	-2.4087610	0.7705880
C	4.9006680	0.5316380	0.0712270
H	5.8885820	0.9720740	0.0089640
C	0.9967150	-1.1728130	0.2809990
C	-0.0515000	-0.5557030	-0.2943540
C	3.7730690	1.3048200	-0.2015730
H	3.8855710	2.3503770	-0.4701740
C	1.2497250	1.5764970	-0.3476910
H	1.4768720	2.4705040	-0.9308410
C	0.1613980	0.7496230	-1.0274590
H	0.4654820	0.4957010	-2.0511830
H	-0.7649280	1.3176200	-1.1080750
H	0.8775390	1.9114780	0.6297910
H	0.8720690	-2.1466640	0.7450230
N	-1.3011450	-1.1635370	-0.4170480
H	-1.3095960	-2.1643720	-0.2718350
C	-2.5158740	-0.5229990	-0.1128300
C	-3.7108710	-1.1054090	-0.5508440
C	-2.5685990	0.6609500	0.6297480
C	-4.9295940	-0.5094480	-0.2587670
H	-3.6692640	-2.0240330	-1.1255610
C	-3.7938160	1.2640010	0.8952240
H	-1.6537760	1.0954760	1.0164530
C	-4.9799520	0.6859520	0.4557620
H	-5.8454140	-0.9762170	-0.6019240
H	-3.8176440	2.1838790	1.4677100
H	-5.9314860	1.1552440	0.6721280

31

3g' rK G -689.008941

C	2.3883760	-0.6615310	-0.0309690
C	3.4972970	-1.4867100	-0.3336040
C	4.7693130	-0.9567390	-0.3485130
H	5.6184930	-1.5822130	-0.5911020
C	2.5918010	0.7072500	0.2932820

H	3.3285210	-2.5313000	-0.5677280
C	4.9592130	0.3977710	-0.0503560
H	5.9589500	0.8142460	-0.0641120
C	1.0755820	-1.1901880	-0.0535600
C	-0.0575370	-0.3577600	-0.0187500
C	3.8779400	1.2176450	0.2738490
H	4.0442640	2.2596280	0.5209250
C	1.4075540	1.5181020	0.7347450
H	1.5986460	2.5813660	0.5931230
C	0.1209680	1.1303090	0.0011240
H	0.1699580	1.4755170	-1.0382300
H	-0.7355770	1.6112680	0.4723910
H	1.2649020	1.3546940	1.8087330
H	0.9357010	-2.2606380	-0.1606760
N	-1.2536760	-0.9367000	-0.0313380
H	-1.2792220	-1.9480680	0.0819370
C	-2.5577350	-0.3798730	-0.0785140
C	-2.8597640	0.8007120	-0.7507590
C	-4.7187060	-0.7387220	0.5274860
C	-4.1846590	1.2177640	-0.7317020
H	-2.1120010	1.3552050	-1.2975610
C	-5.1326150	0.4464530	-0.0741190
H	-5.4311420	-1.3854860	1.0268010
H	-4.4680730	2.1296250	-1.2414350
H	-6.1731840	0.7391400	-0.0419640
N	-3.4542530	-1.1512170	0.5258110

31

3g' N G -689.201973

C	2.3821920	-0.6444990	-0.0405000
C	3.4562340	-1.4140010	-0.4988490
C	4.7306380	-0.8660270	-0.6000460
H	5.5520500	-1.4740250	-0.9606410
C	2.6080070	0.6939580	0.3317240
H	3.2846950	-2.4472710	-0.7821700
C	4.9480600	0.4608340	-0.2421750
H	5.9380520	0.8935570	-0.3223160
C	1.0323080	-1.1965350	0.0589870
C	-0.0472190	-0.3978290	0.1759440
C	3.8842830	1.2321390	0.2247990
H	4.0503350	2.2649420	0.5141120
C	1.4431650	1.4676470	0.8977110
H	1.6233880	2.5412610	0.8204160
C	0.1326270	1.1059190	0.1988580
H	0.1526940	1.4907180	-0.8270390
H	-0.7058340	1.5794820	0.7111820
H	1.3515350	1.2279590	1.9643670
H	0.9096300	-2.2736260	0.0027170
N	-1.3131600	-0.9477230	0.3509170
H	-1.3519980	-1.8934800	0.7065670
C	-2.5617710	-0.4200530	0.0762980
C	-2.7709280	0.6902150	-0.7587670
C	-4.8140110	-0.6590830	0.4266320
C	-4.0693160	1.1293710	-0.9481940
H	-1.9484070	1.1701740	-1.2670410
C	-5.1251530	0.4542800	-0.3407840
H	-5.6019140	-1.2382760	0.8983420
H	-4.2566280	1.9849720	-1.5861830
H	-6.1522230	0.7658340	-0.4720560
N	-3.5719970	-1.0912840	0.6424010

33

3u' rK G -673.140556

C	2.1702200	-0.3940840	-0.4375850
C	3.1330060	-0.9307710	-1.3235760
C	4.4662120	-0.6084900	-1.1783400
H	5.2021840	-1.0123650	-1.8615200
C	2.5846010	0.4571430	0.6178680
H	2.8063510	-1.5870940	-2.1220240
C	4.8639340	0.2462310	-0.1448080
H	5.9104070	0.5018120	-0.0318110
C	0.7957420	-0.7022020	-0.6124340

C	-0.2225790	0.0039790	0.0658610
C	3.9273720	0.7692180	0.7466940
H	4.2502240	1.4200180	1.5510560
C	1.5466500	0.9199530	1.5967230
H	1.8732660	1.8301260	2.0995320
C	0.1855780	1.1636650	0.9401950
H	0.2226550	2.0609390	0.3119170
H	-0.5483750	1.3351630	1.7240010
H	1.4333980	0.1486240	2.3668130
H	0.5433270	-1.4272550	-1.3730190
C	-2.6149050	0.5772690	0.3208220
C	-2.0067060	-1.5044940	-0.7613270
C	-3.5141800	-0.2103550	1.2696840
H	-3.1805680	0.8376460	-0.5774560
H	-2.2501470	1.4913150	0.7746930
C	-2.9388710	-2.2104740	0.2270330
H	-2.5513950	-1.2188810	-1.6634150
H	-1.1925510	-2.1722240	-1.0194210
H	-4.3757730	0.3966840	1.5415090
H	-2.9573280	-0.4771000	2.1767410
H	-3.3769320	-3.0815240	-0.2571620
H	-2.3584170	-2.5354570	1.0996580
N	-1.5039920	-0.2788260	-0.1213050
O	-3.9986930	-1.3705430	0.6271120

33

3u' N G -673.317406

C	2.3412220	-0.6506080	0.1143030
C	3.4113530	-1.5217730	-0.1020530
C	4.7061750	-1.0329860	-0.2436840
H	5.5278010	-1.7182890	-0.4148020
C	2.5812250	0.7324780	0.2010960
H	3.2218170	-2.5882660	-0.1652140
C	4.9407890	0.3360660	-0.1683600
H	5.9462350	0.7238690	-0.2811590
C	0.9646990	-1.1457510	0.2327620
C	-0.0882810	-0.3278010	0.1261390
C	3.8784760	1.2104800	0.0565040
H	4.0614730	2.2780140	0.1238490
C	1.4168810	1.6388860	0.5208980
H	1.6386630	2.6630750	0.2151670
C	0.1170200	1.1533380	-0.1211300
H	0.1345010	1.3371010	-1.2032310
H	-0.7246340	1.7234900	0.2794560
H	1.2833570	1.6489730	1.6102150
H	0.8002670	-2.2106890	0.3614300
C	-2.0308610	-0.5860040	1.5283840
C	-2.3000880	-0.3960270	-0.8498370
C	-3.3836840	-1.2764790	1.5912440
H	-2.1723930	0.4952400	1.6919640
H	-1.3799490	-0.9738980	2.3140220
C	-3.6400770	-1.1019800	-0.7197680
H	-2.4708760	0.6912450	-0.8046970
H	-1.8463180	-0.6361790	-1.8142210
H	-3.8906670	-1.0427720	2.5273610
H	-3.2411820	-2.3630980	1.5200780
H	-4.3374290	-0.7445730	-1.4772810
H	-3.4982990	-2.1840300	-0.8420910
N	-1.4143280	-0.8580910	0.2232980
O	-4.2291730	-0.8353130	0.5420680

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3v' rK G -637.220993

C	2.1281640	-0.3804840	-0.4609770
C	3.0912160	-0.9112610	-1.3495310
C	4.4332350	-0.6603330	-1.1505720
H	5.1696250	-1.0594910	-1.8361490
C	2.5497330	0.3886920	0.6522550
H	2.7590820	-1.5059520	-2.1928270
C	4.8390560	0.1154240	-0.0598690
H	5.8922450	0.3151920	0.0953810
C	0.7459690	-0.6146460	-0.6897040

C	-0.2609280	0.1022250	-0.0025090
C	3.9010530	0.6301380	0.8348540
H	4.2288440	1.2185720	1.6841020
C	1.5045040	0.8425490	1.6274820
H	1.8573540	1.7043410	2.1939410
C	0.1787050	1.1910530	0.9469230
H	0.2810880	2.1182250	0.3715210
H	-0.5703320	1.3579500	1.7174080
H	1.3299610	0.0334320	2.3457220
H	0.4867580	-1.2898520	-1.4920030
C	-2.6197660	0.7632780	0.2841920
C	-2.0948090	-1.2856120	-0.9277560
C	-3.4444650	0.0084390	1.3268550
H	-3.2444210	1.0121320	-0.5781270
H	-2.2027160	1.6886980	0.6646980
C	-2.9143190	-2.1068510	0.0735640
H	-2.7252600	-0.9208040	-1.7419050
H	-1.2981070	-1.8875870	-1.3472730
H	-4.2391680	0.6671240	1.6807480
H	-2.8058960	-0.2327640	2.1822570
H	-3.3310030	-2.9653540	-0.4558100
H	-2.2364590	-2.4888070	0.8428710
N	-1.5479690	-0.1061560	-0.2329320
C	-4.0202220	-1.2676270	0.7125580
H	-4.5415700	-1.8519930	1.4723500
H	-4.7563410	-0.9972360	-0.0518370

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3v' N G -637.394134

C	2.3255550	-0.6537120	0.1245520
C	3.3893230	-1.5366800	-0.0756210
C	4.6900390	-1.0617100	-0.2107320
H	5.5062550	-1.7565010	-0.3692480
C	2.5789630	0.7276920	0.2015610
H	3.1900870	-2.6018530	-0.1313280
C	4.9376480	0.3055640	-0.1453130
H	5.9477100	0.6826320	-0.2532560
C	0.9432500	-1.1342740	0.2359090
C	-0.1021300	-0.3082300	0.1116290
C	3.8819010	1.1919340	0.0633500
H	4.0745730	2.2582620	0.1230260
C	1.4204130	1.6474870	0.5031790
H	1.6551130	2.6673740	0.1924220
C	0.1228310	1.1686860	-0.1481660
H	0.1543730	1.3411010	-1.2318280
H	-0.7176290	1.7510800	0.2369780
H	1.2760570	1.6667670	1.5910800
H	0.7680370	-2.1964650	0.3731450
C	-2.0483550	-0.5327580	1.5061560
C	-2.2912060	-0.3635470	-0.8994000
C	-3.3877810	-1.2522050	1.6316240
H	-2.2050910	0.5530150	1.6378950
H	-1.3589810	-0.8663810	2.2838880
C	-3.6318460	-1.0898120	-0.8576840
H	-2.4728130	0.7237240	-0.8441210
H	-1.7735800	-0.5665270	-1.8400990
H	-3.8367660	-1.0145280	2.5991710
H	-3.2083390	-2.3316820	1.6039610
H	-4.2591890	-0.7399330	-1.6811700
H	-3.4575820	-2.1605680	-1.0029570
N	-1.4345650	-0.8222350	0.2010440
C	-4.3213630	-0.8576170	0.4870280
H	-5.2571170	-1.4184850	0.5427220
H	-4.5749540	0.2050410	0.5805050

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3f' rK G -705.051192

C	2.3719570	-0.6610210	-0.0334240
C	3.4869720	-1.4774820	-0.3412920
C	4.7540560	-0.9377000	-0.3578700
H	5.6077080	-1.5551860	-0.6048980
C	2.5656600	0.7093460	0.2948060

H	3.3252070	-2.5224280	-0.5784750
C	4.9338610	0.4178410	-0.0554460
H	5.9303890	0.8418640	-0.0704240
C	1.0648900	-1.2001760	-0.0538590
C	-0.0729790	-0.3764270	-0.0101900
C	3.8475350	1.2291270	0.2741240
H	4.0070670	2.2714390	0.5238750
C	1.3765250	1.5107340	0.7398330
H	1.5589030	2.5754630	0.5983950
C	0.0928870	1.1127700	0.0063140
H	0.1425540	1.4561120	-1.0333490
H	-0.7673090	1.5902310	0.4752020
H	1.2367420	1.3449670	1.8137880
H	0.9328490	-2.2713580	-0.1634080
N	-1.2681930	-0.9621850	-0.0104140
H	-1.2911340	-1.9734340	0.1050780
C	-2.5628380	-0.3964450	-0.0514950
C	-2.8778610	0.7595640	-0.7669030
C	-4.7157220	-0.6380640	0.5760280
H	-2.1425500	1.2864430	-1.3612810
C	-5.0336270	0.5475920	-0.0864070
H	-5.4735220	-1.2116890	1.0956900
H	-6.0459100	0.9330270	-0.0804330
N	-3.4764710	-1.1114990	0.5906650
N	-4.1195740	1.2318420	-0.7684640

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3f'-N G -705.248185

C	2.3714440	-0.6460290	-0.0274600
C	3.4458380	-1.4212440	-0.4739610
C	4.7184290	-0.8715600	-0.5874940
H	5.5409820	-1.4832420	-0.9389270
C	2.5929060	0.6993190	0.3204500
H	3.2763450	-2.4598330	-0.7381920
C	4.9321920	0.4620160	-0.2533650
H	5.9207690	0.8960600	-0.3431610
C	1.0227770	-1.2005640	0.0845940
C	-0.0560940	-0.4022480	0.1890430
C	3.8675930	1.2389270	0.2019460
H	4.0315790	2.2771240	0.4722200
C	1.4272080	1.4808580	0.8741910
H	1.6041930	2.5530940	0.7750520
C	0.1164020	1.1019790	0.1848190
H	0.1326480	1.4690230	-0.8475260
H	-0.7218800	1.5816940	0.6925190
H	1.3384930	1.2619990	1.9454210
H	0.9029280	-2.2788550	0.0504390
N	-1.3233890	-0.9545150	0.3768170
H	-1.3604150	-1.8888730	0.7627330
C	-2.5639690	-0.4342250	0.0902740
C	-2.7821560	0.6609570	-0.7730110
C	-4.8102980	-0.5985660	0.4011710
H	-1.9630560	1.1345540	-1.2979610
C	-5.0213350	0.5140820	-0.4005090
H	-5.6437460	-1.1240880	0.8546570
H	-6.0175770	0.8973150	-0.5832780
N	-3.5931740	-1.0732360	0.6525820
N	-3.9975640	1.1313450	-0.9983140

30
3i'-rK G -705.067272

C	2.3578550	-0.6585740	0.0396550
C	3.4413910	-1.5296960	-0.2317980
C	4.7165120	-1.0258550	-0.3583060
H	5.5457630	-1.6858260	-0.5770500
C	2.5936140	0.7322950	0.2191530
H	3.2476660	-2.5888340	-0.3544810
C	4.9364540	0.3495190	-0.2064600
H	5.9394180	0.7452670	-0.3093850
C	1.0398300	-1.1628360	0.1107890
C	-0.0828540	-0.3153100	0.1104790
C	3.8832260	1.2161370	0.0856930

H	4.0746040	2.2743020	0.2196660
C	1.4446110	1.5977720	0.6433460
H	1.6379630	2.6394840	0.3884850
C	0.1035290	1.1686590	0.0443980
H	0.0403580	1.4511760	-1.0135060
H	-0.7176020	1.6762630	0.5424400
H	1.3733380	1.5431060	1.7356430
H	0.8844990	-2.2363340	0.0867130
N	-1.2804180	-0.9031630	0.1156380
H	-1.3007350	-1.9152590	0.2157850
C	-2.5814410	-0.3699520	-0.0033000
C	-4.7773070	-0.8319920	0.1325530
C	-3.9909620	1.3143320	-0.4640860
C	-5.0711550	0.4796360	-0.2218350
H	-5.5616700	-1.5534070	0.3309630
H	-4.1289470	2.3492870	-0.7550280
H	-6.0895040	0.8287490	-0.3107350
N	-3.5258790	-1.2698250	0.2455420
N	-2.7283350	0.8923290	-0.3623080

30
3i'-N G -705.263909

C	2.3433840	-0.6464950	0.0021050
C	3.3889620	-1.4492790	-0.4635420
C	4.6616370	-0.9194820	-0.6500190
H	5.4617190	-1.5525670	-1.0152340
C	2.5934710	0.7064660	0.2953160
H	3.1966980	-2.4936860	-0.6862330
C	4.9034620	0.4218890	-0.3711960
H	5.8917360	0.8408400	-0.5183200
C	0.9921130	-1.1785500	0.1779610
C	-0.0727040	-0.3645250	0.2992580
C	3.8676510	1.2260830	0.1031120
H	4.0543720	2.2706470	0.3310910
C	1.4625810	1.5169910	0.8778120
H	1.6469320	2.5837040	0.7377750
C	0.1089600	1.1368030	0.2773560
H	0.0291460	1.4923940	-0.7542730
H	-0.6958510	1.6164930	0.8327030
H	1.4314160	1.3334530	1.9592850
H	0.8569650	-2.2556360	0.1573100
N	-1.3427850	-0.9104670	0.5079540
H	-1.3819280	-1.8615070	0.8481430
C	-2.5654930	-0.4107000	0.1395660
C	-4.8118010	-0.7002270	0.1918200
C	-3.8407090	1.1533840	-0.8818290
C	-4.9971840	0.4785040	-0.5231690
H	-5.6592480	-1.3030480	0.5036960
H	-3.8864180	2.0754680	-1.4530590
H	-5.9794850	0.8390470	-0.7903840
N	-3.6133750	-1.1537410	0.5347680
N	-2.6203980	0.7191940	-0.5711060

39
3c'-rK G -826.726466

C	0.1033870	0.3292950	-2.1854100
C	-0.2938810	0.9310420	-3.4029450
C	-0.4352340	0.1663130	-4.5417090
H	-0.7285370	0.6276520	-5.4760010
C	0.3267060	-1.0738030	-2.1311220
H	-0.4711910	2.0001370	-3.4277520
C	-0.1951910	-1.2115810	-4.4849710
H	-0.3048950	-1.8128790	-5.3793850
C	0.2670010	1.1184430	-1.0194420
C	0.8714520	0.5976460	0.1409290
C	0.1776110	-1.8220500	-3.2872410
H	0.3453180	-2.8925710	-3.2560480
C	0.6424860	-1.7033340	-0.8029110
H	1.1723080	-2.6449730	-0.9455830
C	1.4703660	-0.7761410	0.0871810
H	2.4689980	-0.6411230	-0.3487720
H	1.6078890	-1.2033310	1.0760960

H	-0.3016840	-1.9372900	-0.2973560
H	-0.0434670	2.1581450	-1.0323850
N	0.9867700	1.3756480	1.2069050
H	0.6647290	2.3355000	1.1100440
C	1.5164360	1.0224920	2.4861490
C	2.5503050	1.7795220	3.0185800
C	0.9625810	-0.0314730	3.2161650
C	3.0639100	1.4763260	4.2750250
H	2.9661410	2.6027810	2.4500260
C	1.4722620	-0.3395160	4.4616750
H	0.1253640	-0.5910280	2.8152940
C	2.5292600	0.4080170	4.9992580
H	3.8737950	2.0734830	4.6691230
H	1.0568580	-1.1499070	5.0472450
O	2.9559620	0.0294610	6.2210750
C	4.0257680	0.7614850	6.8263500
H	4.9071740	0.7106810	6.1797290
H	3.7289370	1.8093870	6.9327540
C	4.2993340	0.1320590	8.1728620
H	5.1129420	0.6643710	8.6674910
H	3.4133930	0.1846270	8.8070330
H	4.5886750	-0.9130820	8.0553120

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3c¹-N G -826.914882

C	0.1145790	0.3532290	-2.0913940
C	-0.1232280	1.0902170	-3.2576670
C	0.1784640	0.5621640	-4.5093850
H	-0.0092070	1.1488890	-5.4013020
C	0.6545010	-0.9435080	-2.2034200
H	-0.5436860	2.0874820	-3.1767200
C	0.7235770	-0.7144690	-4.6145980
H	0.9641030	-1.1290640	-5.5863340
C	-0.1871070	0.8929740	-0.7675340
C	0.3253620	0.3338270	0.3512950
C	0.9560490	-1.4597020	-3.4580570
H	1.3724210	-2.4594590	-3.5334770
C	0.8242150	-1.7424060	-0.9346970
H	1.5465450	-2.5472040	-1.0833400
C	1.2571880	-0.8540320	0.2307900
H	2.2801810	-0.5035600	0.0549010
H	1.2653250	-1.4215290	1.1627100
H	-0.1371480	-2.2096270	-0.6859100
H	-0.8150990	1.7761150	-0.7001710
N	-0.0378820	0.7630100	1.6163450
H	-0.7985780	1.4279710	1.6521000
C	0.7642360	0.6951850	2.7747580
C	2.1539620	0.7509360	2.7284230
C	0.1396900	0.5928600	4.0252550
C	2.9174660	0.6672780	3.8939810
H	2.6578840	0.8784930	1.7785230
C	0.8876660	0.5423720	5.1868010
H	-0.9425950	0.5492860	4.0751770
C	2.2857390	0.5657380	5.1310000
H	3.9954150	0.7049950	3.8157650
H	0.4062050	0.4671640	6.1545270
O	2.9336560	0.4894530	6.3251170
C	4.3587260	0.5139750	6.3142600
H	4.7326350	-0.3239850	5.7163390
H	4.7034730	1.4467560	5.8554200
C	4.8276610	0.4091710	7.7481000
H	5.9180450	0.4249000	7.7818380
H	4.4498760	1.2466820	8.3364370
H	4.4797220	-0.5221450	8.1974110

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3b-rK G -830.068531

C	-0.1160200	0.2814710	-2.1020870
C	-0.8572320	0.9008690	-3.1344930
C	-0.5828660	0.6104340	-4.4542920
H	-1.1413690	1.0923230	-5.2462730
C	0.8894770	-0.6684920	-2.4254030

H	-1.6291990	1.6150580	-2.8727500
C	0.4240350	-0.3095380	-4.7660450
H	0.6415130	-0.5360900	-5.8026510
C	-0.3715250	0.6014490	-0.7448810
C	0.5058790	0.2080750	0.2817840
C	1.1469950	-0.9462390	-3.7568840
H	1.9117550	-1.6698260	-4.0141290
C	1.5697980	-1.3983140	-1.3014960
H	2.5317510	-1.7913900	-1.6295000
C	1.7739190	-0.5112030	-0.0708090
H	2.5393990	0.2422370	-0.2867270
H	2.1232970	-1.1026310	0.7752860
H	0.9466620	-2.2556830	-1.0235450
N	0.1896930	0.5078070	1.5357810
C	0.9518330	0.3036180	2.7177770
C	0.2905290	-0.1464040	3.8550650
C	3.0041650	0.4052570	3.9525460
C	1.0003050	-0.3336480	5.0345290
H	-0.7707080	-0.3622170	3.8138790
C	2.3703070	-0.0701490	5.1089570
H	4.0604930	0.6452470	3.9736840
H	0.4625630	-0.6940240	5.9008640
C	2.3136640	0.5994910	2.7680440
H	2.8214360	1.0070270	1.9036970
C	3.1833640	-0.2651530	6.3885470
C	3.7837490	1.0857710	6.8148620
H	2.9935960	1.8161940	7.0055160
H	4.3636540	0.9582610	7.7325450
H	4.4488030	1.4918740	6.0500060
C	4.3179930	-1.2678480	6.1165470
H	3.9131740	-2.2346820	5.8073360
H	4.9922540	-0.9127680	5.3345950
H	4.9053270	-1.4153950	7.0264420
C	2.3272190	-0.8013080	7.5396650
H	1.5216970	-0.1097260	7.7989040
H	1.8888560	-1.7724950	7.2965170
H	2.9552960	-0.9292470	8.4238150
H	-0.7283000	0.9196260	1.6825420
H	-1.2359920	1.2082260	-0.4969520

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3b¹-N G -830.255723

C	-0.0760620	0.3785080	-2.1018580
C	-0.6155590	1.1763410	-3.1171540
C	-0.2944180	0.9462050	-4.4507550
H	-0.7191830	1.5764220	-5.2235070
C	0.7906570	-0.6752440	-2.4518490
H	-1.2876240	1.9862970	-2.8527880
C	0.5730260	-0.0872770	-4.7908140
H	0.8299550	-0.2678500	-5.8277000
C	-0.3899140	0.6109600	-0.6948790
C	0.3601970	0.0738240	0.2926180
C	1.1079170	-0.8937480	-3.7864990
H	1.7773640	-1.7081410	-4.0451510
C	1.2874820	-1.5669200	-1.3409490
H	2.1872100	-2.1007480	-1.6522980
C	1.5643670	-0.7726050	-0.0648600
H	2.4337150	-0.1253930	-0.2251790
H	1.8086400	-1.4480100	0.7561740
H	0.5184690	-2.3200710	-1.1278970
N	0.0101390	0.2280300	1.6226950
C	0.8248770	0.1172870	2.7557680
C	0.2377190	-0.2177210	3.9781650
C	2.9555880	0.2467800	3.8887740
C	1.0032100	-0.3101600	5.1347040
H	-0.8285740	-0.4125410	4.0174620
C	2.3830530	-0.0939890	5.1196470
H	4.0200000	0.4459680	3.8263290
H	0.4996310	-0.5696880	6.0571770
C	2.2013490	0.3694350	2.7304410
H	2.6793620	0.6861630	1.8129520

C	3.2619240	-0.2007830	6.3675390
C	3.9390790	1.1545690	6.6334600
H	3.1898500	1.9331460	6.7982350
H	4.5701430	1.0897180	7.5242520
H	4.5694320	1.4595680	5.7953510
C	4.3423710	-1.2718410	6.1415780
H	3.8848400	-2.2461270	5.9514410
H	4.9814360	-1.0233920	5.2915300
H	4.9773060	-1.3564460	7.0279150
C	2.4523870	-0.5869660	7.6092580
H	1.6861440	0.1584580	7.8370710
H	1.9655740	-1.5576900	7.4850010
H	3.1211410	-0.6542390	8.4705140
H	-0.9265860	0.5664250	1.7918120
H	-1.2263980	1.2593320	-0.4529120

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3d'-rK G -1009.997314

C	0.2780400	0.3982690	-2.1123570
C	0.0179790	1.0718410	-3.3303800
C	-0.0708620	0.3633860	-4.5083110
H	-0.2582010	0.8773710	-5.4420670
C	0.4134570	-1.0181350	-2.1021900
H	-0.0942360	2.1496590	-3.3205770
C	0.0848660	-1.0280490	-4.4929860
H	0.0165730	-1.5851050	-5.4193490
C	0.3961510	1.1293810	-0.9072930
C	0.8711580	0.5280240	0.2742070
C	0.3190730	-1.7085010	-3.2980450
H	0.4201030	-2.7875330	-3.3018020
C	0.5720920	-1.7175310	-0.7813900
H	1.0544820	-2.6846550	-0.9200120
C	1.3726550	-0.8834760	0.2191250
H	2.4164790	-0.8082450	-0.1122760
H	1.3811760	-1.3532280	1.1987240
H	-0.4257760	-1.9088640	-0.3707060
H	0.1535880	2.1866610	-0.8992380
N	0.9620220	1.2623460	1.3735760
H	0.7254960	2.2482890	1.2938180
C	1.3712210	0.8234340	2.6723670
C	0.6448100	-0.1639240	3.3293320
C	2.8524180	1.0414520	4.5408860
C	1.0390600	-0.5619780	4.5994380
H	-0.2260990	-0.6035390	2.8587440
C	2.1395140	0.0414620	5.1955070
H	3.7100040	1.5012130	5.0159750
H	0.4867360	-1.3317340	5.1218470
C	2.4676570	1.4381240	3.2693100
H	3.0149980	2.2071720	2.7392150
C	2.5507250	-0.3417890	6.5877980
F	2.1490350	0.5698030	7.4876720
F	3.8829350	-0.4323540	6.7036430
F	2.0345980	-1.5169490	6.9640980

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3d'-N G -1010.191382

C	0.2270250	0.3548320	-2.0182520
C	-0.2904460	1.0173020	-3.1348410
C	-0.6533660	0.3088980	-4.2753090
H	-1.0490880	0.8357660	-5.1355090
C	0.3656860	-1.0458230	-2.0506680
H	-0.4018710	2.0961900	-3.1060820
C	-0.5032830	-1.0738820	-4.3102390
H	-0.7799110	-1.6307700	-5.1974860
C	0.6215010	1.0854310	-0.8110480
C	1.4021700	0.5153510	0.1214210
C	0.0025300	-1.7429740	-3.1968500
H	0.1125760	-2.8224380	-3.2177320
C	0.8517810	-1.7391750	-0.8008440
H	1.2479670	-2.7268400	-1.0420580
C	1.9006830	-0.8981310	-0.0776040
H	2.8145980	-0.8330940	-0.6820880

H	2.1852900	-1.3595910	0.8677230
H	-0.0049240	-1.8874490	-0.1299780
H	0.3221860	2.1246350	-0.7141570
N	1.9415570	1.2487210	1.1859560
H	2.0258790	2.2452060	1.0386820
C	1.9068460	0.8460470	2.5171510
C	1.1228390	-0.2313000	2.9508080
C	2.6595460	1.1860110	4.7904490
C	1.1319500	-0.6092970	4.2856740
H	0.4860900	-0.7554490	2.2489670
C	1.9003230	0.0922810	5.2068860
H	3.2566590	1.7364820	5.5077680
H	0.5262820	-1.4464100	4.6100150
C	2.6703410	1.5548880	3.4588590
H	3.2774110	2.3895630	3.1284870
C	1.8705320	-0.2707200	6.6542360
F	1.0271270	0.5085410	7.3601420
F	3.0743690	-0.1341450	7.2360840
F	1.4750710	-1.5363640	6.8577410

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3m'-rK G -787.436285

C	-1.6712580	1.2725110	-0.0864520
C	-2.6689550	2.2486670	-0.3206950
C	-3.9887570	1.8641340	-0.3695330
C	-2.0234590	-0.0799030	0.1216650
H	-2.3797170	3.2813460	-0.4701930
C	-4.3493590	0.5262060	-0.1681110
H	-5.3951370	0.2533080	-0.2043080
C	-0.3045890	1.6519840	-0.0401990
C	0.7284020	0.6968030	-0.0439240
C	-3.3724180	-0.4397290	0.0913270
C	-0.9571930	-1.0805120	0.4623240
H	-1.2713640	-2.0789010	0.1628520
C	0.3825800	-0.7527860	-0.2006750
H	0.3139920	-0.9610090	-1.2742760
H	1.1748070	-1.3809510	0.2055950
H	-0.8324010	-1.0993270	1.5511060
N	1.9822670	1.1177480	0.0645240
C	3.1827820	0.3569260	-0.0086920
C	4.1897830	0.6439540	0.9112760
C	4.5675360	-1.3015860	-1.0485970
C	5.3838870	-0.0604580	0.8514810
H	4.0284740	1.4021940	1.6681620
C	5.5720810	-1.0373420	-0.1228110
H	4.7187160	-2.0456470	-1.8201530
H	6.1665510	0.1535760	1.5680230
H	6.5050850	-1.5849140	-0.1665780
C	3.3687810	-0.6013710	-1.0029170
H	2.6036370	-0.7765080	-1.7476950
H	-4.7644800	2.5945370	-0.5599690
O	-3.6409930	-1.7419920	0.3332220
C	-4.9981230	-2.1649600	0.2953840
H	-4.9819890	-3.2306690	0.5054250
H	-5.5883220	-1.6500500	1.0572620
H	-5.4331460	-1.9922280	-0.6919770
H	-0.0484920	2.7061310	-0.0411460
H	2.1123220	2.1093660	0.2489490

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3m'-N G -787.625098

C	-1.6713240	1.2478650	-0.0605160
C	-2.6334630	2.1911810	-0.4512520
C	-3.9566210	1.8093910	-0.5993050
C	-2.0573640	-0.0763480	0.1855750
H	-2.3321190	3.2156710	-0.6385910
C	-4.3554100	0.4953200	-0.3574190
H	-5.3942030	0.2204400	-0.4752760
C	-0.2696680	1.6235670	0.1089040
C	0.7077580	0.6949000	0.1774540
C	-3.4010430	-0.4415230	0.0456180
C	-1.0132410	-1.0520720	0.6673540

H	-1.3177300	-2.0738560	0.4428500
C	0.3499200	-0.7690630	0.0364680
H	0.3120890	-1.0346420	-1.0257120
H	1.1159290	-1.3923580	0.4998920
H	-0.9318040	-0.9728910	1.7590440
N	2.0195080	1.0551290	0.4418090
C	3.1922200	0.3599570	0.1345120
C	4.3413190	0.6243980	0.8930370
C	4.4714730	-1.2179300	-1.1768210
C	5.5352340	-0.0228680	0.6115640
H	4.2828500	1.3373820	1.7080560
C	5.6076740	-0.9591210	-0.4180460
H	4.5152710	-1.9276250	-1.9946780
H	6.4121780	0.1981160	1.2085870
H	6.5378330	-1.4711460	-0.6299800
C	3.2751890	-0.5562070	-0.9203010
H	2.4177100	-0.7321340	-1.5555140
H	-4.6989630	2.5371960	-0.9056740
O	-3.6943770	-1.7392270	0.3362810
C	-5.0405100	-2.1603260	0.1964050
H	-5.0555440	-3.2135450	0.4654560
H	-5.6998160	-1.6032480	0.8677130
H	-5.3855960	-2.0423650	-0.8344910
H	-0.0241780	2.6797860	0.1566300
H	2.1503500	1.9867420	0.8100420

36
3l'-rK G -787.442690

C	-1.5398960	0.7495380	0.3613190
C	-2.6693740	1.5945270	0.4919960
C	-3.9391090	1.1374990	0.2325730
H	-4.7826750	1.8061440	0.3263810
C	-1.7393930	-0.6175670	-0.0085070
H	-2.5196940	2.6266580	0.7865120
C	-4.1161560	-0.2045250	-0.1591480
C	-0.2412900	1.2423150	0.5915430
C	0.8978020	0.4955730	0.2524870
C	-3.0061820	-1.0694900	-0.2667060
H	-3.1897910	-2.1001120	-0.5463150
C	-0.5443030	-1.5296980	-0.0140850
H	-0.7276910	-2.3949200	-0.6504740
C	0.7240710	-0.8086640	-0.4703420
H	0.6450500	-0.5511200	-1.5342000
H	1.5926540	-1.4522510	-0.3606200
H	-0.3953290	-1.9008350	1.0061400
H	-0.1152370	2.2427930	0.9918790
N	2.1028930	1.0090230	0.4748230
H	2.1402230	1.9520210	0.8510980
C	3.3670570	0.3868160	0.2210420
C	4.2520520	1.0043810	-0.6562790
C	3.7105950	-0.7879450	0.8843240
C	5.4939180	0.4233980	-0.8854670
H	3.9638480	1.9221020	-1.1544340
C	4.9505680	-1.3649370	0.6396750
H	3.0183900	-1.2312670	1.5906100
C	5.8410890	-0.7616270	-0.2440890
H	6.1871890	0.8963720	-1.5694640
H	5.2238120	-2.2799310	1.1498420
H	6.8083670	-1.2123800	-0.4278380
O	-5.2962490	-0.7501100	-0.4400350
C	-6.4715030	0.0562740	-0.3451970
H	-6.4163790	0.8957770	-1.0403810
H	-7.2954400	-0.5958150	-0.6177090
H	-6.6056500	0.4176920	0.6757470

36
3l'-N G -787.624701

C	-1.4930690	0.7470720	0.1765960
C	-2.5986260	1.5425670	0.4657700
C	-3.8986710	1.0416370	0.4019490
H	-4.7314370	1.6928270	0.6294540
C	-1.7066220	-0.6029210	-0.1749470

H	-2.4474770	2.5806260	0.7430180
C	-4.0973470	-0.2888900	0.0399810
C	-0.1240260	1.2650700	0.2347430
C	0.8947840	0.6075000	-0.3450460
C	-2.9938780	-1.1033780	-0.2431680
H	-3.1741600	-2.1387880	-0.5117860
C	-0.4937770	-1.4717430	-0.4040520
H	-0.7592030	-2.3527920	-0.9904610
C	0.6262880	-0.6855730	-1.0819020
H	0.3323420	-0.4193470	-2.1054240
H	1.5289200	-1.2909820	-1.1633250
H	-0.1351550	-1.8257410	0.5715800
H	0.0430180	2.2302170	0.7038920
N	2.1730840	1.1620650	-0.4696640
H	2.2196740	2.1652730	-0.3511570
C	3.3511300	0.4827610	-0.1178160
C	4.5824660	1.0246220	-0.5072110
C	3.3363290	-0.7051910	0.6207930
C	5.7678530	0.3861830	-0.1723560
H	4.5954240	1.9463060	-1.0785610
C	4.5297350	-1.3503170	0.9297280
H	2.3940490	-1.1098680	0.9718200
C	5.7509910	-0.8127730	0.5382800
H	6.7112510	0.8228740	-0.4786110
H	4.4997760	-2.2723180	1.4986280
H	6.6769960	-1.3151410	0.7884120
O	-5.3140990	-0.8864450	-0.0620150
C	-6.4567120	-0.0956220	0.2186780
H	-6.5285320	0.7508400	-0.4700930
H	-7.3156400	-0.7478650	0.0828260
H	-6.4374440	0.2729610	1.2481510

36
3j'-rK G -787.434866

C	1.6330180	-0.3417090	0.2052930
C	2.8320900	-1.0743590	0.2794160
C	4.0473920	-0.4560800	0.0328260
C	1.6596070	1.0502610	-0.0930950
H	2.8158890	-2.1322820	0.5126100
C	4.0712220	0.9131760	-0.2812310
H	5.0065880	1.4181510	-0.4804260
C	0.3925330	-0.9871330	0.4361410
C	-0.8314230	-0.3496330	0.1516720
C	2.8840000	1.6441680	-0.3339540
H	2.9293120	2.7026900	-0.5623190
C	0.3745770	1.8282070	-0.0511890
H	0.4543310	2.7254530	-0.6645770
C	-0.8139780	0.9894840	-0.5223120
H	-0.7127550	0.7753580	-1.5940500
H	-1.7495090	1.5249010	-0.3877320
H	0.1937620	2.1549010	0.9790700
H	0.3818620	-2.0066770	0.8066010
N	-1.9600200	-0.9972200	0.3941010
H	-1.8801130	-1.9513870	0.7366290
C	-3.2947570	-0.5077120	0.2176990
C	-3.7220210	0.6122750	0.9254050
C	-5.4602120	-0.7532470	-0.7772990
C	-5.0279650	1.0557440	0.7599930
H	-3.0443020	1.1149780	1.6054400
C	-5.8954650	0.3759960	-0.0904500
H	-6.1353690	-1.2851700	-1.4354920
H	-5.3691070	1.9260780	1.3059520
H	-6.9137250	0.7233940	-0.2125170
C	-4.1541470	-1.2036660	-0.6256210
H	-3.7988570	-2.0770680	-1.1588450
O	5.1462570	-1.2360300	0.1110740
C	6.4116360	-0.6352770	-0.1350660
H	7.1435330	-1.4299780	-0.0213950
H	6.4629680	-0.2333940	-1.1499730
H	6.6162880	0.1566670	0.5896070

36

3jⁱ N G -787.624702

C	1.5881610	-0.3332880	0.0583000
C	2.7758990	-1.0326590	0.2481340
C	4.0095650	-0.3801080	0.1792360
C	1.6301310	1.0550080	-0.1937920
H	2.7660600	-2.0990870	0.4452470
C	4.0586150	0.9871910	-0.0835660
H	4.9993480	1.5160850	-0.1481370
C	0.2903660	-1.0082740	0.1209370
C	-0.8189430	-0.4291020	-0.3748780
C	2.8607450	1.6851190	-0.2634110
H	2.9003460	2.7521760	-0.4577840
C	0.3198100	1.7942500	-0.3108080
H	0.4604350	2.7405550	-0.8360580
C	-0.7288890	0.9376930	-1.0157630
H	-0.4432560	0.7800330	-2.0637710
H	-1.6973470	1.4368120	-1.0266300
H	-0.0443310	2.0328830	0.6974370
H	0.2517750	-2.0194690	0.5146960
N	-2.0249820	-1.1172050	-0.5016860
H	-1.9576480	-2.1234250	-0.4253880
C	-3.2722660	-0.5881500	-0.1223280
C	-3.3847820	0.5307890	0.7089380
C	-5.6840920	-0.7352130	-0.2100060
C	-4.6404110	1.0243160	1.0479540
H	-2.4909880	0.9991840	1.1053030
C	-5.7959630	0.3975040	0.5939780
H	-6.5751550	-1.2388980	-0.5658690
H	-4.7110890	1.8955510	1.6885910
H	-6.7709490	0.7810790	0.8674030
C	-4.4360690	-1.2200490	-0.5749320
H	-4.3474880	-2.0884270	-1.2182960
O	5.1036050	-1.1643870	0.3763740
C	6.3749480	-0.5409290	0.3127050
H	7.1050480	-1.3252620	0.4959390
H	6.5502930	-0.1028130	-0.6739620
H	6.4726370	0.2343750	1.0778800

32

3nⁱ-rK G -772.201579

C	-1.9728220	0.7800670	0.2078550
C	-3.0936940	1.6410950	0.2985910
C	-4.3577520	1.1791530	0.0135530
H	-5.2306300	1.8161160	0.0627150
C	-2.1601980	-0.5856850	-0.1491480
H	-2.9435990	2.6758470	0.5816380
C	-4.4993730	-0.1575820	-0.3524410
C	-0.6739050	1.2694090	0.4773200
C	0.4742820	0.5101740	0.1802920
C	-3.4317830	-1.0434200	-0.4328110
H	-3.6161300	-2.0749650	-0.7064360
C	-0.9720390	-1.5051920	-0.1248410
H	-1.1440850	-2.3655640	-0.7707060
C	0.3132520	-0.7923900	-0.5452850
H	0.2621680	-0.5316000	-1.6102020
H	1.1751210	-1.4405660	-0.4143120
H	-0.8554730	-1.8838170	0.8968670
H	-0.5550630	2.2691420	0.8809500
N	1.6674120	1.0156430	0.4515410
H	1.6956230	1.9582570	0.8319810
C	2.9384830	0.3864750	0.2473070
C	3.8612600	1.0060230	-0.5883220
C	3.2446430	-0.7941020	0.9177850
C	5.1071750	0.4175480	-0.7701130
H	3.5992870	1.9284260	-1.0920340
C	4.4908080	-1.3760150	0.7219850
H	2.5210670	-1.2371790	1.5919360
C	5.4200810	-0.7729650	-0.1211430
H	5.8308110	0.8896220	-1.4224050
H	4.7377120	-2.2950390	1.2381060
H	6.3914500	-1.2285410	-0.2673250

F -5.7196780 -0.6117910 -0.6326590

32

3nⁱ-N G -772.390739

C	-1.9260040	0.7330970	0.2189120
C	-3.0335770	1.5364370	0.5033200
C	-4.3263880	1.0274110	0.4405910
H	-5.1933840	1.6396700	0.6534540
C	-2.1282950	-0.6183400	-0.1231690
H	-2.8818730	2.5758610	0.7725080
C	-4.4896830	-0.2991310	0.0890810
C	-0.5605690	1.2595410	0.2777800
C	0.4634250	0.6056480	-0.2994080
C	-3.4175500	-1.1307780	-0.1906660
H	-3.5988820	-2.1672020	-0.4516490
C	-0.9111700	-1.4814190	-0.3451880
H	-1.1711010	-2.3680070	-0.9253360
C	0.2028690	-0.6929570	-1.0289910
H	-0.0939870	-0.4321650	-2.0529510
H	1.1079610	-1.2941670	-1.1089960
H	-0.5512400	-1.8256310	0.6334170
H	-0.4014660	2.2284620	0.7410470
N	1.7333100	1.1694200	-0.4274960
H	1.7757560	2.1705320	-0.2905560
C	2.9251150	0.4900830	-0.1175400
C	4.1401380	1.0309140	-0.5541000
C	2.9363550	-0.6928470	0.6283390
C	5.3373880	0.3952610	-0.2571770
H	4.1312640	1.9487290	-1.1315820
C	4.1400400	-1.3358520	0.8986530
H	2.0067350	-1.0953200	1.0143500
C	5.3459680	-0.7991360	0.4607700
H	6.2691680	0.8301100	-0.5993060
H	4.1313920	-2.2543830	1.4737250
H	6.2806920	-1.2993600	0.6810330
F	-5.7379940	-0.8079020	0.0173720

29

3oⁱ-rK G -721.099738

C	2.3711280	-0.6679120	0.1468240
C	3.5255710	-1.4732460	0.2469030
C	4.7565280	-0.8911060	0.0506750
H	5.6700630	-1.4669470	0.1060320
C	2.5414990	0.7199720	-0.1213880
H	3.4277970	-2.5304850	0.4634240
C	4.8077890	0.4784340	-0.2300480
H	5.7639210	0.9839620	-0.3983090
C	1.0757450	-1.2012710	0.3424280
C	-0.0780090	-0.4437280	0.0609050
C	1.3357510	1.6123270	-0.1251110
H	1.5371320	2.4827100	-0.7471900
C	0.0858360	0.8833430	-0.6177730
H	0.1993900	0.6413010	-1.6825720
H	-0.7915430	1.5155900	-0.5293570
H	1.1744940	1.9694980	0.8984850
N	-1.2638130	-0.9870710	0.2992150
C	-2.5528290	-0.4012750	0.1552360
C	-2.8578620	0.8451120	0.6986950
C	-4.6677920	-0.6504180	-0.5701750
H	-2.1258740	1.4126260	1.2628860
C	-4.9744000	0.6191550	-0.0824390
H	-5.4170690	-1.2589390	-1.0614940
H	-5.9685780	1.0329150	-0.2000680
N	-3.4481730	-1.1644180	-0.4484940
N	-4.0752590	1.3578100	0.5634800
N	3.7318650	1.2696070	-0.3063750
H	0.9676520	-2.2199210	0.6989080
H	-1.2868750	-1.9663460	0.5774020

29

3oⁱ-N G -721.302571

C	2.3274950	-0.6261350	0.1876630
C	3.4612500	-1.3986050	0.4289030

C	4.7136160	-0.7992210	0.3774790
H	5.6164420	-1.3691740	0.5548700
C	2.5133560	0.7442520	-0.0824320
H	3.3599170	-2.4559150	0.6492790
C	4.7867350	0.5567650	0.0893690
H	5.7480380	1.0574050	0.0361560
C	0.9730360	-1.1772700	0.2220190
C	-0.0602740	-0.5017360	-0.3058230
C	1.2887850	1.6033400	-0.2668050
H	1.5605590	2.5055870	-0.8140170
C	0.1758700	0.8345530	-0.9741250
H	0.4619700	0.6228770	-2.0123420
H	-0.7342760	1.4312640	-1.0233270
H	0.9367320	1.9110900	0.7267390
N	-1.3250200	-1.0882360	-0.4379990
C	-2.5290690	-0.4952060	-0.1264180
C	-2.6200750	0.7192370	0.5864990
C	-4.7949520	-0.5875270	-0.2068060
H	-1.7292820	1.2130670	0.9598380
C	-4.8858340	0.6348440	0.4424660
H	-5.6879380	-1.1273730	-0.5026260
H	-5.8452590	1.0889430	0.6571210
N	-3.6256810	-1.1557330	-0.4970620
N	-3.7875740	1.2790090	0.8522140
N	3.7104340	1.3209600	-0.1324540
H	0.8288840	-2.1720060	0.6311870
H	-1.3737980	-2.0897750	-0.5688620

for Table S8

32
3a'' G -673.146759

C	1.0833150	0.4544870	0.6546640
C	-0.2727630	-0.1859110	0.4511090
C	-0.3632360	-1.6776580	0.7214270
C	0.9237100	-2.2394720	1.3413310
C	2.1250030	-1.8047130	0.5406420
C	2.1962830	-0.4497660	0.1822160
H	-1.2312800	-1.8746290	1.3594710
H	1.1040290	1.4287010	0.1626820
H	1.1988620	0.6284390	1.7359700
H	-0.5596530	-2.1817300	-0.2330770
N	-1.2450500	0.5473100	0.0739650
C	-2.5208640	-0.0359130	-0.1144000
C	-3.4906990	0.0653690	0.8891930
C	-2.8482770	-0.6447520	-1.3312950
C	-4.7648010	-0.4608880	0.6841720
H	-3.2351030	0.5553590	1.8241350
C	-4.1259080	-1.1646130	-1.5301120
H	-2.0967730	-0.7035090	-2.1135510
C	-5.0892240	-1.0782160	-0.5243480
H	-5.5079850	-0.3830810	1.4719460
H	-4.3688910	-1.6372840	-2.4769780
H	-6.0837430	-1.4821050	-0.6828930
C	3.2702720	0.0128350	-0.5771500
C	3.1338520	-2.6779250	0.1345320
C	4.2133100	-2.2102600	-0.6166890
H	4.9947220	-2.8965800	-0.9277650
C	4.2811380	-0.8641330	-0.9735280
H	5.1151620	-0.4977100	-1.5637980
H	3.3159150	1.0615280	-0.8593730
H	3.0736880	-3.7288420	0.4061070
H	1.0176090	-1.8709090	2.3718690
H	0.8690890	-3.3297380	1.3970850

32
3a' G -673.146978

C	1.0448060	0.0396180	-1.0642860
C	-0.0395250	-0.2853090	-0.3234360
C	0.1376760	-1.1167110	0.9315750
C	1.4504770	-0.7455180	1.6226620

C	2.6152290	-0.7978400	0.6631860
C	2.3908840	-0.3667560	-0.6611500
H	-0.7071950	-0.9644210	1.6082970
H	0.9290930	0.5956080	-1.9918920
H	0.1602780	-2.1829760	0.6715790
N	-1.3014210	0.2019870	-0.6389220
H	-1.3214000	0.9772500	-1.2880200
C	-2.5392300	-0.3919790	-0.3682450
C	-3.6819240	0.4236490	-0.3420350
C	-2.6838860	-1.7698370	-0.1556570
C	-4.9348670	-0.1266980	-0.0979080
H	-3.5744700	1.4921410	-0.5076770
C	-3.9418280	-2.3068850	0.1143220
H	-1.8225340	-2.4237580	-0.2278750
C	-5.0740520	-1.4950630	0.1451420
H	-5.8064410	0.5204880	-0.0846380
H	-4.0343620	-3.3758160	0.2807010
H	-6.0511510	-1.9210310	0.3464460
C	3.4677900	-0.3339690	-1.5572880
C	3.8912930	-1.1951470	1.0528640
C	4.9579970	-1.1673610	0.1505080
H	5.9474050	-1.4813130	0.4676990
C	4.7421780	-0.7312070	-1.1563710
H	5.5645230	-0.7027850	-1.8647870
H	3.2986000	0.0011670	-2.5776070
H	4.0551600	-1.5257430	2.0759000
H	1.3669280	0.2767200	2.0188400
H	1.6259830	-1.4087200	2.4745940

31

3a'BnC G -672.345640

C	1.1081860	-0.3474430	-1.4145860
C	-0.0749640	-0.6124300	-0.7151300
C	-0.0194080	-1.0240860	0.7190450
C	1.3318390	-1.1234160	1.3112990
C	2.4636820	-0.8600860	0.6081500
C	2.3479730	-0.4610080	-0.7939040
H	-0.6244610	-0.3306580	1.3238990
H	1.0590560	-0.0486630	-2.4572670
N	-1.2661860	-0.5063100	-1.3008940
H	-1.2925700	-0.2256850	-2.2760560
C	-2.5202470	-0.7620090	-0.6467890
C	-3.1777380	0.2814110	0.0025790
C	-3.0537990	-2.0494250	-0.6709260
C	-4.3905090	0.0271550	0.6408050
H	-2.7419070	1.2758910	0.0015440
C	-4.2670860	-2.2938380	-0.0298400
H	-2.5229990	-2.8426390	-1.1886410
C	-4.9328800	-1.2579550	0.6255860
H	-4.9108850	0.8335150	1.1464350
H	-4.6915090	-3.2919790	-0.0456170
H	-5.8776790	-1.4517570	1.1224170
C	3.5585060	-0.1902380	-1.5083330
C	3.7755740	-0.9656550	1.2145250
C	4.8883210	-0.6976140	0.4915840
H	5.8735470	-0.7739590	0.9367700
C	4.7679140	-0.3049260	-0.8892930
H	5.6734580	-0.0948170	-1.4498880
H	3.4949130	0.1073800	-2.5497340
H	3.8343730	-1.2637700	2.2567870
H	1.3901430	-1.4218310	2.3545940
H	-0.5361750	-1.9884380	0.8445850

31

3a'AC G -672.331599

C	1.1073400	-0.2087050	-1.2195620
C	-0.0833650	-0.4810360	-0.4982220
C	0.0601300	-0.9474260	0.7918880
C	1.3699930	-1.2024630	1.4065580
C	2.5764750	-0.8941830	0.6022480
C	2.4047460	-0.3817000	-0.7129450
H	-0.8173500	-1.1449010	1.4002570

H	1.0089950	0.1635840	-2.2388740
N	-1.2965570	-0.2660160	-1.1288780
H	-1.3043060	0.4621540	-1.8309670
C	-2.5547780	-0.5774150	-0.5570490
C	-3.5498280	0.4005490	-0.4941020
C	-2.8222760	-1.8745860	-0.1066420
C	-4.8069090	0.0805030	0.0167490
H	-3.3380440	1.4065450	-0.8448100
C	-4.0722250	-2.1788000	0.4254350
H	-2.0607220	-2.6446980	-0.1928460
C	-5.0699550	-1.2047550	0.4873160
H	-5.5770660	0.8439590	0.0555930
H	-4.2722170	-3.1865980	0.7746930
H	-6.0458190	-1.4487450	0.8931760
C	3.5387500	-0.0727720	-1.5144060
C	3.8670450	-1.0913170	1.0921030
C	4.9616400	-0.7820300	0.2956810
H	5.9626520	-0.9352410	0.6856660
C	4.8014810	-0.2719480	-1.0096810
H	5.6750190	-0.0406110	-1.6081970
H	3.3901880	0.3161590	-2.5168710
H	4.0114120	-1.4833210	2.0940760
H	1.4089800	-0.6566710	2.3646250
H	1.4007330	-2.2575660	1.7312840

31

3a'BnR G -672.517180

C	1.0061340	-0.0891580	-1.0840440
C	-0.0568260	-0.1987600	-0.2542980
C	0.0913030	-0.6991350	1.1620350
C	1.4767560	-1.1382250	1.5003770
C	2.5612960	-1.0007610	0.6266210
C	2.3492230	-0.4623820	-0.6865890
H	-0.2280080	0.1183520	1.8323630
H	0.8624240	0.3036580	-2.0886050
N	-1.3086840	0.3089330	-0.6026990
H	-1.3131780	0.9292350	-1.4028930
C	-2.5286150	-0.3657380	-0.3761890
C	-3.7079660	0.3855870	-0.2930610
C	-2.5959500	-1.7599910	-0.2655480
C	-4.9313000	-0.2478810	-0.0963770
H	-3.6520700	1.4671730	-0.3768730
C	-3.8218190	-2.3845400	-0.0410590
H	-1.6938200	-2.3534080	-0.3819330
C	-4.9947060	-1.6355610	0.0438130
H	-5.8373340	0.3472370	-0.0373070
H	-3.8591270	-3.4659970	0.0472390
H	-5.9476290	-2.1266840	0.2104820
C	3.4359160	-0.3306780	-1.5569220
C	3.8828290	-1.3859600	0.9933980
C	4.9372450	-1.2431280	0.1129340
H	5.9372880	-1.5407270	0.4126680
C	4.7189610	-0.7121390	-1.1718780
H	5.5484360	-0.6007810	-1.8625250
H	3.2664610	0.0761060	-2.5508360
H	4.0475680	-1.7953750	1.9867000
H	1.6421240	-1.5567280	2.4887070
H	-0.6204500	-1.5078290	1.3760090

31

3a'AR G -672.521984

C	1.0694640	-0.2025920	-1.2133250
C	-0.0555830	-0.4024970	-0.3794750
C	0.1031260	-0.8549090	0.9081300
C	1.4375160	-1.2430310	1.4609420
C	2.6136180	-0.9127180	0.5750310
C	2.4024850	-0.4137030	-0.7322080
H	-0.7578070	-0.9582880	1.5594410
H	0.9229780	0.1370010	-2.2345610
N	-1.3111110	-0.0771100	-0.9312980
H	-1.3173500	0.7581600	-1.5004700
C	-2.5604920	-0.4818730	-0.4582430

C	-3.6563900	0.3850660	-0.5887690
C	-2.7743810	-1.7638580	0.0736930
C	-4.9297410	-0.0180680	-0.1962430
H	-3.5023170	1.3789750	-1.0007190
C	-4.0492130	-2.1501300	0.4772510
H	-1.9450290	-2.4584620	0.1540220
C	-5.1370110	-1.2851590	0.3482270
H	-5.7621310	0.6699700	-0.3090720
H	-4.1931890	-3.1458930	0.8858650
H	-6.1278420	-1.5949460	0.6627370
C	3.5234640	-0.1400050	-1.5474740
C	3.9171240	-1.1150160	1.0279940
C	5.0146570	-0.8380360	0.2153220
H	6.0212650	-1.0010900	0.5865850
C	4.8115080	-0.3491110	-1.0811690
H	5.6614710	-0.1322420	-1.7206250
H	3.3602100	0.2410650	-2.5521840
H	4.0725680	-1.4976590	2.0343000
H	1.5755130	-0.7689780	2.4432310
H	1.4467830	-2.3249130	1.6763600

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3a G -671.978394

C	1.0385870	-0.0135270	-1.0620650
C	-0.0345960	-0.2290000	-0.2219460
C	0.1783210	-0.8777480	1.0318920
C	1.4295070	-1.3037300	1.3886230
C	2.5518970	-1.0967710	0.5387040
C	2.3475170	-0.4262130	-0.7005440
H	0.8864020	0.4807630	-2.0186510
N	-1.3009510	0.2609790	-0.5534470
H	-1.3170090	0.9975530	-1.2451420
C	-2.5263040	-0.3775790	-0.3281190
C	-3.7031400	0.3789200	-0.4466960
C	-2.6257470	-1.7421850	-0.0211180
C	-4.9459850	-0.2149310	-0.2578240
H	-3.6307760	1.4370130	-0.6834160
C	-3.8766120	-2.3215190	0.1850180
H	-1.7314360	-2.3530070	0.0383030
C	-5.0440180	-1.5686000	0.0701200
H	-5.8433050	0.3882150	-0.3570740
H	-3.9336040	-3.3794050	0.4230980
H	-6.0138290	-2.0282460	0.2276200
C	3.4667260	-0.2065590	-1.5508580
C	3.8588920	-1.5232910	0.8925130
C	4.9224800	-1.2975860	0.0517260
H	5.9187110	-1.6262720	0.3295310
C	4.7207130	-0.6319190	-1.1839930
H	5.5660260	-0.4581630	-1.8426050
H	3.3127220	0.3034110	-2.4981240
H	4.0031670	-2.0315590	1.8424440
H	1.5813720	-1.7925520	2.3473270
H	-0.6592890	-1.0098830	1.7088580

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PQ G -688.525440

C	-10.5706420	-6.0788010	0.5928610
C	-9.1834100	-6.0915030	0.6269380
C	-8.4642050	-4.8920880	0.6406450
C	-9.1236870	-3.6458360	0.6253050
C	-10.5240820	-3.6563500	0.5860440
C	-11.2360670	-4.8522700	0.5702960
C	-6.9863200	-4.9739620	0.6617260
C	-8.3523650	-2.3731560	0.6501340
C	-6.9424500	-2.3810090	0.6308060
C	-6.1860110	-3.6531900	0.6054490
C	-6.2119870	-1.1884150	0.6444720
H	-5.1286290	-1.2478200	0.6277520
C	-6.8651210	0.0353930	0.6824640
C	-8.2602830	0.0576280	0.7090070
C	-8.9909940	-1.1269440	0.6933130
H	-11.1290210	-7.0084470	0.5802450

H	-8.6293570	-7.0244100	0.6405020
H	-11.0829240	-2.7292840	0.5625660
H	-12.3204680	-4.8229620	0.5383580
H	-6.2993790	0.9605780	0.6950490
H	-8.7880020	1.0053040	0.7440420
H	-10.0713640	-1.0606090	0.7199540
O	-6.3769780	-6.0210090	0.7129290
O	-4.9760020	-3.7087200	0.5507680

26
H2PQ G -689.726658

C	-10.5389300	-6.0777760	0.5688510
C	-9.1596000	-6.0786980	0.5851890
C	-8.4455350	-4.8614460	0.6197710
C	-9.1359250	-3.6236610	0.6382670
C	-10.5483450	-3.6594560	0.6207070
C	-11.2366150	-4.8564420	0.5866320
C	-7.0076390	-4.8671820	0.6524460
C	-8.3781710	-2.3779340	0.6701130
C	-6.9590410	-2.4279300	0.6732940
C	-6.3026660	-3.7051750	0.6871440
C	-6.2123950	-1.2284060	0.6667950
H	-5.1283530	-1.2711910	0.6343310
C	-6.8481630	-0.0037010	0.6771600
C	-8.2525700	0.0559550	0.6915620
C	-8.9960330	-1.1085640	0.6836200
H	-11.0842350	-7.0156210	0.5419830
H	-8.6037310	-7.0097560	0.5723460
H	-11.1150800	-2.7358040	0.6324050
H	-12.3217570	-4.8518320	0.5731060
H	-6.2640860	0.9109100	0.6685300
H	-8.7558430	1.0171420	0.7018430
H	-10.0772260	-1.0327820	0.6861590
O	-6.3846470	-6.0736080	0.6547640
O	-4.9275430	-3.8128660	0.6676400
H	-5.4289700	-5.9136300	0.6882880
H	-4.5363440	-3.2871280	1.3783240

26
H2PQ' G -689.716792

H	-0.0484150	0.4620520	0.7130800
H	-1.2113360	-0.6238030	2.6964030
C	-0.9830380	-2.8431330	-1.8255840
C	-1.1183900	-2.0250300	-0.7057370
C	0.0101040	-1.5040530	-0.0775570
C	1.2969830	-1.7946040	-0.5632390
C	1.4163770	-2.6254070	-1.6848030
C	0.2878170	-3.1403690	-2.3158280
C	-0.1438070	-0.5709770	1.1017840
C	2.4882760	-1.2755530	0.1560940
C	2.3564940	-0.7916610	1.4737560
C	1.0108980	-0.6947500	2.0782930
C	3.4701300	-0.3923500	2.2171660
H	3.3187590	-0.0393180	3.2325350
C	4.7360200	-0.4306690	1.6474330
C	4.8779330	-0.8766310	0.3308290
C	3.7726110	-1.2969790	-0.4030390
H	-1.8649940	-3.2520250	-2.3078550
H	-2.0984060	-1.7913140	-0.3039700
H	2.3972160	-2.8979310	-2.0590610
H	0.4035810	-3.7850470	-3.1809560
H	5.6028710	-0.1071020	2.2133150
H	5.8605500	-0.8971110	-0.1297730
H	3.9181310	-1.6358240	-1.4226230
O	0.8010720	-0.6329960	3.2772910
O	-1.3774840	-0.7267510	1.7450970

56
3a'PQ vdW G -1361.669506

C	1.1006530	0.1677260	1.1150990
C	2.2308400	-0.2756370	0.5177760
C	2.3232890	-1.7197080	0.0674110
C	0.9638310	-2.2056840	-0.4394350

C	-0.1412010	-1.9037350	0.5429900
C	-0.0650570	-0.6974240	1.2737110
H	3.0775740	-1.8220900	-0.7171330
H	1.0395450	1.1879080	1.4880860
H	2.6409890	-2.3486120	0.9092830
N	3.2772470	0.5912660	0.2363720
H	3.0472040	1.5758610	0.2567870
C	4.6360760	0.2874940	0.1085600
C	5.4526850	1.1624180	-0.6259380
C	5.2171280	-0.8354430	0.7141070
C	6.8134510	0.9115190	-0.7590260
H	5.0065790	2.0341610	-1.0967460
C	6.5779130	-1.0907820	0.5521380
H	4.6146570	-1.4923980	1.3306640
C	7.3858540	-0.2241760	-0.1817600
H	7.4278870	1.6013260	-1.3294110
H	7.0097860	-1.9679090	1.0244280
H	8.4458290	-0.4243460	-0.2960430
C	-1.1164450	-0.3591170	2.1390940
C	-1.2395220	-2.7450760	0.7167320
C	-2.2708460	-2.4088730	1.5949960
H	-3.1225800	-3.0714640	1.7140790
C	-2.2095800	-1.2059700	2.3008950
H	-3.0153830	-0.9266180	2.9734300
H	-1.0677670	0.5799890	2.6863790
H	-1.2926960	-3.6693100	0.1453760
H	0.7343770	-1.7018890	-1.3895370
H	1.0051950	-3.2793620	-0.6450930
C	-5.2138210	-1.6497050	-0.6520910
C	-3.9823650	-1.5913800	-1.2876280
C	-3.1383080	-0.4921460	-1.1007120
C	-3.5125500	0.5786580	-0.2655020
C	-4.7621640	0.5015780	0.3649590
C	-5.5989020	-0.5935060	0.1759730
C	-1.8345220	-0.5001430	-1.7979070
C	-2.6032570	1.7365500	-0.0547160
C	-1.3332670	1.7766630	-0.6644440
C	-0.8726950	0.6772260	-1.5428960
C	-0.4605030	2.8466780	-0.4480870
H	0.5082130	2.8260240	-0.9376830
C	-0.8295770	3.9001150	0.3776600
C	-2.0860440	3.8753020	0.9846620
C	-2.9585390	2.8115510	0.7699610
H	-5.8667930	-2.5041390	-0.7944070
H	-3.6436640	-2.3952700	-1.9333810
H	-5.0994500	1.2947960	1.0206820
H	-6.5586950	-0.6217150	0.6821280
H	-0.1523580	4.7302510	0.5476040
H	-2.3929600	4.6908110	1.6318260
H	-3.9225160	2.8343990	1.2627760
O	0.2168880	0.6652570	-2.0782880
O	-1.4917680	-1.3751450	-2.5677360

56
3a'Bnc-HPQ-vdW G-1361.633759

C	0.9185760	-0.0085220	1.7276840
C	2.0802090	-0.3444400	1.0428460
C	2.2257870	-1.6860490	0.4011700
C	0.9539070	-2.4456950	0.2869700
C	-0.1981650	-2.0629800	0.9061580
C	-0.2248790	-0.8091270	1.6424230
H	2.6981470	-1.5780440	-0.5814450
H	0.8551480	0.9495560	2.2361000
H	2.9282210	-2.2898400	1.0010150
N	3.1157450	0.5150830	0.9930840
H	2.9499890	1.4468560	1.3558600
C	4.3238160	0.3187620	0.2585940
C	4.5677680	1.0979690	-0.8730790
C	5.2573360	-0.6286110	0.6807620
C	5.7531420	0.9253790	-1.5852980
H	3.8241970	1.8216190	-1.1930060

C	6.4324830	-0.8081580	-0.0462490
H	5.0668920	-1.2073790	1.5794550
C	6.6829190	-0.0310590	-1.1774640
H	5.9433050	1.5310450	-2.4652400
H	7.1574200	-1.5468080	0.2797910
H	7.6018000	-0.1687670	-1.7378810
C	-1.4535900	-0.4100650	2.2520520
C	-1.4115100	-2.8433400	0.8163640
C	-2.5545090	-2.4257800	1.4161980
H	-3.4669810	-3.0063910	1.3344800
C	-2.5745970	-1.1812900	2.1342650
H	-3.5054710	-0.8486350	2.5837960
H	-1.4853330	0.5378690	2.7819130
H	-1.3834230	-3.7635580	0.2397430
H	-0.1065980	-1.6336070	-2.1443410
H	0.9856920	-3.3833410	-0.2626920
C	-5.1692110	-1.1403300	-1.3087290
C	-3.8343900	-1.3445810	-1.5796420
C	-2.8616810	-0.3808100	-1.2070790
C	-3.2704450	0.8103430	-0.5402830
C	-4.6482590	0.9854260	-0.2816480
C	-5.5831050	0.0378740	-0.6529590
C	-1.4841960	-0.5988580	-1.4651200
C	-2.2622160	1.7978500	-0.1720580
C	-0.8963440	1.5464210	-0.4643050
C	-0.4776840	0.3108080	-1.1152750
C	0.0874630	2.4920160	-0.1119170
H	1.1179870	2.2598420	-0.3674460
C	-0.2526290	3.6655860	0.5323490
C	-1.6029030	3.9215150	0.8348580
C	-2.5810530	3.0077160	0.4853760
H	-5.9034790	-1.8857750	-1.5994900
H	-3.5004860	-2.2492470	-2.0779930
H	-4.9929390	1.8828340	0.2208150
H	-6.6345620	0.2025800	-0.4401700
H	0.5118940	4.3888580	0.8003530
H	-1.8824220	4.8415280	1.3390350
H	-3.6128220	3.2380280	0.7276910
O	0.7496580	0.0125160	-1.3445480
O	-1.0782340	-1.7315920	-2.1034150

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3a'-PQ-TS1 G -1361.618084 ifreq -1331.67

C	1.0367930	0.2719990	1.6793850
C	2.1666470	-0.2045000	1.0573790
C	2.2361040	-1.6174920	0.5539130
C	0.8925840	-2.2962730	0.4395020
C	-0.2123630	-1.8051250	1.1720950
C	-0.1678680	-0.4810090	1.7230630
H	2.7734690	-1.6336620	-0.4016320
H	1.0241180	1.2910230	2.0593950
H	2.8560970	-2.2008400	1.2521560
N	3.2492320	0.6114510	0.9059470
H	3.0589670	1.5938980	1.0619600
C	4.4460800	0.3439420	0.2012250
C	4.8676240	1.2551050	-0.7736430
C	5.2383670	-0.7701580	0.4959940
C	6.0639070	1.0459450	-1.4542740
H	4.2465150	2.1166770	-1.0016350
C	6.4224190	-0.9842390	-0.2062550
H	4.9431070	-1.4517210	1.2861120
C	6.8416910	-0.0795130	-1.1813060
H	6.3807610	1.7585900	-2.2089880
H	7.0281770	-1.8542940	0.0261700
H	7.7692430	-0.2465530	-1.7186380
C	-1.3489070	0.0562380	2.3028870
C	-1.4274560	-2.5458340	1.2719920
C	-2.5442280	-2.0048010	1.8521370
H	-3.4656670	-2.5763470	1.9029610
C	-2.5099290	-0.6765160	2.3562240
H	-3.4068620	-0.2415500	2.7864630

H	-1.3221520	1.0746380	2.6832260
H	-1.4561660	-3.5458360	0.8458370
H	0.3224010	-1.9301940	-0.8901060
H	0.9316720	-3.3714050	0.2671340
C	-4.5491140	-2.0844640	-1.5674590
C	-3.1762160	-1.9563610	-1.6334140
C	-2.5444470	-0.7528270	-1.2561520
C	-3.3200850	0.3415440	-0.8005090
C	-4.7195050	0.1861980	-0.7548570
C	-5.3275080	-1.0007890	-1.1278670
C	-1.1074680	-0.6407570	-1.3437310
C	-2.6562740	1.5960620	-0.4037910
C	-1.2547510	1.7191740	-0.5193940
C	-0.4302660	0.6023520	-1.0229440
C	-0.6034680	2.8921760	-0.1145360
H	0.4762780	2.9367660	-0.2196180
C	-1.3234640	3.9546160	0.4095710
C	-2.7144450	3.8462120	0.5268610
C	-3.3667990	2.6881830	0.1255570
H	-5.0254570	-3.0147790	-1.8603770
H	-2.5538500	-2.7776350	-1.9739740
H	-5.3475490	1.0059070	-0.4254150
H	-6.4082470	-1.0889980	-1.0822370
H	-0.8164630	4.8605830	0.7259390
H	-3.2916020	4.6697980	0.9355940
H	-4.4432830	2.6379150	0.2408750
O	0.8085820	0.6763650	-1.0977980
O	-0.3665890	-1.6372010	-1.7370470

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3a'-PQ-TS2 G -1361.615330 ifreq = -1263.42

C	-1.1920240	1.2960640	0.5569960
C	-2.3522590	0.9967930	1.3964580
C	-3.6292480	0.6520210	0.8078100
C	-3.7215610	0.4976710	-0.5984130
H	-0.3721150	0.4635900	0.7733740
H	-0.6281780	2.1681530	0.8885280
C	0.9883350	1.8158000	-1.4068900
C	2.1457320	1.1649210	-1.8513450
C	1.1101910	3.0170440	-0.6946110
C	3.4022520	1.6843230	-1.5520900
H	2.0511960	0.2405710	-2.4148240
C	2.3713030	3.5147390	-0.3768080
H	0.2217720	3.5762740	-0.4201140
C	3.5240510	2.8509620	-0.7978910
H	4.2894160	1.1600650	-1.8936380
H	2.4501340	4.4401950	0.1850220
H	4.5044810	3.2442570	-0.5505290
C	-4.9588720	0.1229050	-1.1641520
C	-4.7768150	0.4500770	1.6025960
C	-5.9822980	0.0924750	1.0274710
H	-6.8582500	-0.0588670	1.6498100
C	-6.0710850	-0.0783670	-0.3669170
H	-7.0162470	-0.3637030	-0.8178720
H	-5.0278490	0.0000970	-2.2418180
H	-4.6982170	0.5775600	2.6792760
H	-1.8953430	-0.2545000	1.8692890
H	-2.3802060	1.4887490	2.3679660
C	-1.0036850	-2.6987560	-1.8549850
C	-1.1028760	-2.1451500	-0.5848800
C	0.0467230	-1.7254760	0.0995810
C	1.3245260	-1.8673610	-0.4888780
C	1.3984090	-2.4382950	-1.7657340
C	0.2527410	-2.8432340	-2.4459120
C	-0.1030300	-1.0807180	1.4044660
C	2.5234420	-1.3923310	0.2356810
C	2.3955090	-0.7028510	1.4602260
C	1.0768530	-0.5273240	2.1184230
C	3.5239350	-0.1971760	2.1192450
H	3.3751100	0.3300400	3.0559970
C	4.7912790	-0.3780870	1.5885650

C	4.9330530	-1.0861600	0.3904410
C	3.8193060	-1.5827890	-0.2723780
H	-1.8986020	-3.0136120	-2.3822570
H	-2.0702160	-2.0255510	-0.1060200
H	2.3572970	-2.5616710	-2.2561570
H	0.3438720	-3.2739350	-3.4378390
H	5.6630560	0.0153790	2.1006070
H	5.9203910	-1.2498350	-0.0302960
H	3.9701540	-2.1228560	-1.1997750
O	0.9434700	0.0558390	3.1890210
O	-1.2185640	-1.1745010	2.0548350
C	-2.5696740	0.7460990	-1.4228670
C	-1.3712260	1.1510620	-0.9133480
H	-2.6688990	0.6074550	-2.4972970
N	-0.2688740	1.2798580	-1.7388470
H	-0.3078130	0.7491470	-2.5995050

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3a'-PQ-H2O-TS1 G -1438.038607 ifreq = -1312.83

C	0.9406590	0.4571690	1.6468730
C	2.0995490	-0.0582370	1.1059020
C	2.2071180	-1.5202540	0.7844370
C	0.8713540	-2.2097730	0.6575080
C	-0.2532250	-1.6926370	1.3365990
C	-0.2406820	-0.3205930	1.7640700
H	2.8120450	-1.6450780	-0.1203940
H	0.8924880	1.5126890	1.9033250
H	2.7550080	-2.0159330	1.6012970
N	3.1431900	0.7698630	0.8441380
H	2.9209780	1.7575670	0.8813790
C	4.4197460	0.4636090	0.3252330
C	4.9606800	1.3189930	-0.6412360
C	5.1711930	-0.6196490	0.7894410
C	6.2317100	1.0799000	-1.1515340
H	4.3688730	2.1544740	-1.0040490
C	6.4360180	-0.8637380	0.2567860
H	4.7861390	-1.2545110	1.5788710
C	6.9725160	-0.0191300	-0.7132240
H	6.6381950	1.7467450	-1.9050720
H	7.0095400	-1.7107580	0.6195720
H	7.9601760	-0.2102850	-1.1193260
C	-1.4373020	0.2334150	2.3010780
C	-1.4478940	-2.4546860	1.5008430
C	-2.5768670	-1.8926570	2.0320190
H	-3.4837960	-2.4798610	2.1362930
C	-2.5752800	-0.5239370	2.4214540
H	-3.4829900	-0.0783560	2.8168720
H	-1.4388080	1.2805180	2.5934420
H	-1.4484300	-3.4895560	1.1681610
H	0.3666960	-1.8078940	-0.6715070
H	0.9173000	-3.2895310	0.5210950
C	-4.2064810	-2.5544280	-1.5046120
C	-2.8772960	-2.1839240	-1.5462680
C	-2.4791670	-0.8793830	-1.1859410
C	-3.4502450	0.0685740	-0.7822180
C	-4.7999030	-0.3344630	-0.7564330
C	-5.1768580	-1.6199630	-1.1064360
C	-1.0789030	-0.5221000	-1.2298610
C	-3.0312410	1.4341650	-0.4236830
C	-1.6717180	1.8017470	-0.5180960
C	-0.6465040	0.8301180	-0.9452310
C	-1.2528660	3.0916030	-0.1611450
H	-0.1970640	3.3273790	-0.2482520
C	-2.1651560	4.0287680	0.2962000
C	-3.5169380	3.6758940	0.3953770
C	-3.9399450	2.4031050	0.0393040
H	-4.5013080	-3.5608750	-1.7846900
H	-2.1115780	-2.8895340	-1.8520870
H	-5.5716200	0.3677120	-0.4625720
H	-6.2249040	-1.9003020	-1.0775740
H	-1.8374580	5.0249760	0.5752290

H	-4.2428970	4.3994180	0.7530250
H	-4.9927580	2.1645670	0.1358670
O	0.5608380	1.1431210	-0.9963000
O	-0.1690660	-1.3926010	-1.5842110
H	1.8630540	0.1162340	-1.7686730
O	2.5262560	-0.4369730	-2.2283830
H	1.9801440	-1.1222820	-2.6312780

59

3a'-PQ-TS2-H2O G -1438.033201 ifreq = -1282.25

C	1.1631520	0.3598770	1.2790090
C	2.3562660	1.1325930	0.9114630
C	3.6026410	0.4751740	0.5954450
C	3.6366260	-0.9408240	0.5170930
H	0.3313980	0.5867780	0.4846880
H	0.6660580	0.7489160	2.1682060
C	-1.1045630	-1.4879270	1.8666540
C	-2.2630180	-1.9531600	1.2324430
C	-1.2262360	-0.6828210	3.0076260
C	-3.5192330	-1.5824830	1.7041300
H	-2.1688640	-2.5904730	0.3575070
C	-2.4862410	-0.2937580	3.4550380
H	-0.3420700	-0.3924040	3.5646830
C	-3.6391610	-0.7342960	2.8042960
H	-4.4068160	-1.9430210	1.1935640
H	-2.5645490	0.3397540	4.3329590
H	-4.6186120	-0.4303900	3.1584610
C	4.8488380	-1.5744460	0.1673580
C	4.7783030	1.2137130	0.3402560
C	5.9560500	0.5726160	0.0074790
H	6.8548870	1.1494380	-0.1841100
C	5.9881640	-0.8328960	-0.0845880
H	6.9129810	-1.3354150	-0.3498040
H	4.8755700	-2.6590050	0.1038590
H	4.7402780	2.2980460	0.4098110
H	1.9165630	1.5333820	-0.3568840
H	2.4202000	2.1406090	1.3209320
C	0.7894690	-2.2383640	-2.5675510
C	0.9651610	-0.9439170	-2.0962890
C	-0.1417950	-0.1706220	-1.7157500
C	-1.4522180	-0.6944230	-1.8118480
C	-1.6024810	-1.9972840	-2.3031100
C	-0.4999360	-2.7645710	-2.6699570
C	0.0818840	1.1606360	-1.1631510
C	-2.6012320	0.1245940	-1.3722410
C	-2.3947140	1.3782080	-0.7560560
C	-1.0409580	1.9598240	-0.6312560
C	-3.4774360	2.1336140	-0.2833950
H	-3.2686340	3.0892130	0.1863080
C	-4.7749110	1.6703700	-0.4268620
C	-4.9939740	0.4424010	-1.0614290
C	-3.9269550	-0.3148960	-1.5238150
H	1.6503850	-2.8346470	-2.8525240
H	1.9589870	-0.5142220	-2.0130560
H	-2.5884300	-2.4397140	-2.3896530
H	-0.6499460	-3.7744030	-3.0379610
H	-5.6113260	2.2562910	-0.0608660
H	-6.0061880	0.0731320	-1.1941180
H	-4.1376480	-1.2620570	-2.0065130
O	-0.8391550	3.0573490	-0.1051500
O	1.2347550	1.7386370	-1.2782350
H	0.8504700	3.8868480	0.0189940
O	1.6954800	4.3614280	0.1264420
H	2.1988870	4.1223730	-0.6596960
C	2.4544550	-1.7021700	0.8115380
C	1.2796300	-1.1232850	1.1974610
H	2.5083380	-2.7852640	0.7256920
N	0.1499020	-1.8963720	1.3769810
H	0.1666530	-2.7973360	0.9162420

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3a'-HPQ-vdW-H2O G -1438.057971

C	0.7715870	0.3166280	1.8825530
C	1.9592750	-0.1308130	1.3066100
C	2.1198580	-1.5709820	0.9443120
C	0.8568330	-2.3459290	0.9144940
C	-0.3180270	-1.8587110	1.3995330
C	-0.3643670	-0.4911150	1.8984330
H	2.6562410	-1.7105510	0.0024500
H	0.6890350	1.3516230	2.2026400
H	2.7731080	-2.0158570	1.7183680
N	3.0101480	0.6956580	1.1899860
H	2.8982120	1.6333060	1.5596130
C	4.1760660	0.4542110	0.3993650
C	4.0393020	0.2188050	-0.9711910
C	5.4337390	0.4985940	0.9976800
C	5.1804160	0.0032850	-1.7397100
H	3.0417360	0.2121050	-1.4062370
C	6.5710420	0.2989200	0.2151710
H	5.5141850	0.6841810	2.0643420
C	6.4454400	0.0448470	-1.1499610
H	5.0816060	-0.1847400	-2.8039620
H	7.5528770	0.3345050	0.6757590
H	7.3315830	-0.1168180	-1.7550740
C	-1.6198280	0.0124090	2.3667740
C	-1.5327170	-2.6438240	1.3917530
C	-2.6976960	-2.1225660	1.8471330
H	-3.6119020	-2.7055170	1.8275290
C	-2.7377450	-0.7676030	2.3307720
H	-3.6871600	-0.3593470	2.6647780
H	-1.6690140	1.0390980	2.7177670
H	-1.4837610	-3.6531830	0.9939840
H	-0.3126790	-2.2016640	-1.7725010
H	0.9080970	-3.3565840	0.5178940
C	-5.2371830	-1.0639660	-1.0632220
C	-3.9119660	-1.3798630	-1.2732470
C	-2.8918540	-0.4147900	-1.0747600
C	-3.2466900	0.8949360	-0.6500410
C	-4.6141340	1.1860150	-0.4475660
C	-5.5949960	0.2335750	-0.6464820
C	-1.5198950	-0.7665610	-1.2697730
C	-2.1910510	1.8766560	-0.4479170
C	-0.8438900	1.4958490	-0.6695370
C	-0.4846750	0.1424460	-1.0742490
C	0.1914950	2.4361190	-0.4760630
H	1.2102520	2.1073970	-0.6619700
C	-0.0853480	3.7236960	-0.0611610
C	-1.4195680	4.1073130	0.1704930
C	-2.4454170	3.2008170	-0.0232210
H	-6.0055970	-1.8153360	-1.2193710
H	-3.6243290	-2.3770520	-1.5883440
H	-4.9126580	2.1785600	-0.1278610
H	-6.6376920	0.4868540	-0.4829930
H	0.7192190	4.4387450	0.0835450
H	-1.6474080	5.1173910	0.4968540
H	-3.4641310	3.5254590	0.1586110
O	0.7714210	-0.1807960	-1.1947700
O	-1.2699520	-2.0482440	-1.6672470
H	1.3209370	-1.4707990	-1.8013150
O	1.5703400	-2.4149700	-2.0801930
H	1.7857070	-2.3897030	-3.0185790

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3a'-PQ-TS1-PhOH G -1668.971982 ifreq = -1304.26

C	-0.0697850	-0.6447560	-1.8787600
C	-1.2171120	-1.1437680	-1.3003260
C	-1.1535020	-2.3354370	-0.3920250
C	0.2385060	-2.6854520	0.0689380
C	1.3577980	-2.2873680	-0.6934560
C	1.2149570	-1.1871570	-1.6051570
H	-1.8176750	-2.1668550	0.4627550
H	-0.1342840	0.2134460	-2.5433110
H	-1.5510980	-3.2050390	-0.9395510

N	-2.4048670	-0.5376620	-1.5705360
H	-2.3091970	0.3214260	-2.0994480
C	-3.7349770	-0.8159500	-1.2120820
C	-4.6527350	0.2309960	-1.4028540
C	-4.2036600	-2.0467030	-0.7356460
C	-5.9956790	0.0619750	-1.1039270
H	-4.2951460	1.1914650	-1.7641110
C	-5.5565900	-2.1996470	-0.4277110
H	-3.5495210	-2.8971660	-0.6181720
C	-6.4597680	-1.1564920	-0.6036220
H	-6.6792080	0.8928540	-1.2470760
H	-5.8999220	-3.1598210	-0.0551710
H	-7.5084900	-1.2887360	-0.3596120
C	2.3808980	-0.6818590	-2.2460120
C	2.6496870	-2.8554290	-0.4930600
C	3.7481930	-2.3531310	-1.1370460
H	4.7287690	-2.7856420	-0.9651480
C	3.6133520	-1.2393430	-2.0114660
H	4.4937620	-0.8296130	-2.4970420
H	2.2798870	0.1698450	-2.9139030
H	2.7465460	-3.6831970	0.2046820
H	0.5061190	-1.7139870	1.1360500
H	0.3203260	-3.6160560	0.6288560
C	4.9259220	-1.5076360	2.5242170
C	3.5776260	-1.2987330	2.3135470
C	3.1328780	-0.2807390	1.4448140
C	4.0723420	0.5496800	0.7880870
C	5.4413840	0.3172380	1.0252550
C	5.8659880	-0.6926690	1.8721070
C	1.7151210	-0.0983180	1.2259470
C	3.5996810	1.6300490	-0.0950780
C	2.2152360	1.8506990	-0.2616480
C	1.2247900	0.9916810	0.4104160
C	1.7481590	2.8667320	-1.1082680
H	0.6751600	2.9980870	-1.2056360
C	2.6374660	3.6699170	-1.8031810
C	4.0136330	3.4598730	-1.6481640
C	4.4834450	2.4606650	-0.8076270
H	5.2581990	-2.2937740	3.1948750
H	2.8337970	-1.9166830	2.8064020
H	6.1900420	0.9364520	0.5446320
H	6.9277620	-0.8468270	2.0354680
H	2.2736280	4.4531640	-2.4601950
H	4.7222730	4.0811810	-2.1868470
H	5.5549190	2.3258550	-0.7167270
O	-0.0024370	1.1666480	0.2502820
O	0.8302410	-0.8580490	1.8123540
H	-1.2182350	0.3313690	1.1674590
O	-2.0352370	-0.0464220	1.5764880
C	-3.0669170	0.8276630	1.5091890
C	-4.2878970	0.4347910	2.0699380
C	-2.9521660	2.0863100	0.9054570
C	-5.3819810	1.2918190	2.0235720
H	-4.3601410	-0.5479110	2.5263150
C	-4.0583350	2.9354480	0.8682300
H	-2.0020930	2.3827820	0.4713360
C	-5.2778790	2.5487750	1.4227360
H	-6.3265000	0.9721520	2.4547160
H	-3.9605640	3.9103900	0.3986800
H	-6.1340470	3.2147030	1.3884790

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3a'-PQ-TS2-PhOH G -1668.965856 ifreq = -1307.03

C	1.2561850	0.3839310	0.5051960
C	2.4777400	0.5736970	-0.2952720
C	3.6414030	-0.2516010	-0.0979440
C	3.5645100	-1.3501880	0.7967770
H	0.3754180	0.2148310	-0.2497210
H	0.9449840	1.3082660	1.0021980
C	-1.2221010	-0.6908910	2.0738890
C	-2.2046300	-1.5692700	2.5694510

C	-1.6201190	0.5905440	1.6696640
C	-3.5328080	-1.1799580	2.6613640
H	-1.9128470	-2.5707630	2.8763900
C	-2.9625360	0.9632680	1.7505670
H	-0.9159120	1.3210860	1.3012590
C	-3.9275370	0.0944400	2.2471300
H	-4.2653330	-1.8818920	3.0482720
H	-3.2455640	1.9568750	1.4146550
H	-4.9679690	0.3965430	2.3021900
C	4.7017660	-2.1721730	0.9673250
C	4.8512250	0.0039770	-0.7821610
C	5.9519640	-0.8070860	-0.5942580
H	6.8774170	-0.6005160	-1.1216830
C	5.8730610	-1.9072870	0.2852070
H	6.7389100	-2.5459480	0.4286490
H	4.6422100	-3.0168710	1.6484430
H	4.8992450	0.8518240	-1.4606370
H	1.9575970	0.1099300	-1.5106100
H	2.6527310	1.5888290	-0.6482720
C	0.5372320	-3.9386030	-0.4900250
C	0.7755380	-2.7089660	-1.0905050
C	-0.2741750	-1.7997210	-1.2910340
C	-1.5928720	-2.1295380	-0.8955770
C	-1.8065780	-3.3754690	-0.2958970
C	-0.7573960	-4.2673060	-0.0854440
C	0.0315090	-0.4803450	-1.8325670
C	-2.6832260	-1.1592010	-1.1156340
C	-2.4108540	0.1083760	-1.6779100
C	-1.0430610	0.5023110	-2.0609990
C	-3.4389140	1.0397220	-1.8816230
H	-3.1823590	2.0009330	-2.3152110
C	-4.7458570	0.7322600	-1.5402800
C	-5.0283840	-0.5222340	-0.9904610
C	-4.0155850	-1.4486580	-0.7817900
H	1.3561660	-4.6334400	-0.3322150
H	1.7765040	-2.4342160	-1.4095060
H	-2.7995180	-3.6617080	0.0311130
H	-0.9552040	-5.2232220	0.3890870
H	-5.5401010	1.4540060	-1.6992670
H	-6.0476760	-0.7783710	-0.7179900
H	-4.2749000	-2.4060380	-0.3458520
O	-0.8044500	1.6142020	-2.5526010
O	1.2021290	-0.2285220	-2.3295110
H	0.5766640	2.6114490	-2.2224670
O	1.2870880	3.1663070	-1.8296060
C	2.3460020	-1.6065980	1.5027710
C	1.2348870	-0.8139120	1.3885360
H	2.3085410	-2.4796860	2.1512080
N	0.0895350	-1.1827330	2.0583360
H	0.1741800	-2.0830270	2.5141730
C	0.9250830	3.6088150	-0.5994240
C	-0.4001220	3.5901950	-0.1446940
C	1.9388620	4.0943460	0.2353620
C	-0.6928700	4.0449840	1.1418740
H	-1.1866490	3.2204690	-0.7970360
C	1.6318250	4.5399780	1.5177590
H	2.9594070	4.1079350	-0.1355880
C	0.3151030	4.5141340	1.9832020
H	-1.7228200	4.0314520	1.4871490
H	2.4279710	4.9079080	2.1578020
H	0.0784090	4.8607570	2.9834080

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3a'-HPQ G -vdW-PhOH -1668.994439

C	-0.0138110	-0.8142670	-1.6920300
C	-0.8725850	-1.7613860	-1.1256280
C	-0.3393840	-3.0995190	-0.7271780
C	1.1398790	-3.2165010	-0.7275440
C	1.9568300	-2.2495910	-1.2179250
C	1.3624620	-1.0106510	-1.7124040
H	-0.7542420	-3.4145010	0.2389340

H	-0.4193420	0.1415590	-2.0116730
H	-0.7032970	-3.8497850	-1.4484540
N	-2.1579140	-1.4372340	-0.9406310
H	-2.3624930	-0.4415110	-1.0975580
C	-3.1610220	-2.1419730	-0.2338690
C	-3.9542140	-1.4005590	0.6508720
C	-3.4083330	-3.5035060	-0.4251510
C	-4.9753440	-2.0284110	1.3556750
H	-3.7579880	-0.3389260	0.7842310
C	-4.4278570	-4.1241770	0.2952290
H	-2.8403880	-4.0719020	-1.1520710
C	-5.2108360	-3.3941550	1.1873440
H	-5.5834670	-1.4490020	2.0425200
H	-4.6165140	-5.1818640	0.1432540
H	-6.0048060	-3.8832220	1.7416370
C	2.2454090	0.0070820	-2.1996230
C	3.3974680	-2.4060210	-1.2482950
C	4.1866890	-1.4114720	-1.7161730
H	5.2659220	-1.5157460	-1.7243950
C	3.5937220	-0.1839870	-2.1863140
H	4.2476640	0.6112280	-2.5327330
H	1.8191280	0.9447020	-2.5439190
H	3.8186790	-3.3325350	-0.8692470
H	-0.2841770	-1.0298080	1.5969970
H	1.5571030	-4.1513190	-0.3619940
C	4.8155740	-1.6041390	1.9651130
C	3.4415710	-1.5214100	1.9068590
C	2.8095430	-0.3545880	1.4089450
C	3.5949200	0.7491970	0.9748110
C	5.0008140	0.6234940	1.0414810
C	5.6040860	-0.5234480	1.5217960
C	1.3921120	-0.2719180	1.3246890
C	2.9231540	1.9404780	0.4738820
C	1.5020340	1.9889950	0.4496240
C	0.7207020	0.8564500	0.8967150
C	0.8435660	3.1384650	-0.0440450
H	-0.2425360	3.1524750	-0.0465040
C	1.5617910	4.2177960	-0.5151270
C	2.9695540	4.1779160	-0.4993170
C	3.6285180	3.0654980	-0.0125670
H	5.2915620	-2.5014210	2.3495690
H	2.8186290	-2.3474090	2.2360830
H	5.6328590	1.4419360	0.7134560
H	6.6869320	-0.5867780	1.5630550
H	1.0460490	5.0946670	-0.8941120
H	3.5412200	5.0240310	-0.8678030
H	4.7131130	3.0651250	-0.0128160
O	-0.5936910	0.8314180	0.8947360
O	0.6330830	-1.3599230	1.6619220
H	-1.4308760	1.2388320	-0.1289600
O	-2.1567060	1.4009110	-0.8921290
C	-3.2111730	2.1179120	-0.4423330
C	-4.2766510	2.3701440	-1.3167590
C	-3.2675100	2.5998140	0.8740530
C	-5.3822540	3.0941060	-0.8782650
H	-4.2195270	1.9914460	-2.3329000
C	-4.3809460	3.3241640	1.2984530
H	-2.4388670	2.3944190	1.5461250
C	-5.4439670	3.5768420	0.4308640
H	-6.2018190	3.2826820	-1.5656260
H	-4.4145780	3.6930360	2.3195560
H	-6.3070840	4.1409430	0.7683710

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3g' G -689.207895

C	-1.1787270	0.5931090	-0.9816710
C	-2.2594680	1.3848690	-0.2437210
C	-3.6315810	0.7846380	-0.4331300
C	-3.7306660	-0.6209470	-0.4770790
H	-0.1864830	0.9564670	-0.7066680
H	-1.2721660	0.7313900	-2.0649590

C	1.0392580	-1.5315750	-1.2442590
C	2.1504280	-2.3120940	-0.8597520
C	2.2240720	-0.5789290	-2.9563520
C	3.3184830	-2.1956280	-1.5884210
H	2.0799550	-2.9794250	-0.0069610
C	3.3711020	-1.3027870	-2.6656820
H	2.2123760	0.1235330	-3.7863020
H	4.1874050	-2.7872680	-1.3175400
H	4.2692870	-1.1774250	-3.2583830
C	-4.9960540	-1.2140350	-0.5736140
C	-4.7873340	1.5580790	-0.5009500
C	-6.0457700	0.9596890	-0.6060430
C	-6.1472000	-0.4306340	-0.6382110
H	-5.0732590	-2.2980290	-0.6047910
H	-2.0276550	1.3852190	0.8314030
H	-2.2503870	2.4278510	-0.5735230
C	-2.5095890	-1.4266340	-0.4265890
C	-1.2966810	-0.8806570	-0.6585160
H	-2.6047510	-2.4935510	-0.2366440
N	-0.1386890	-1.6516480	-0.5253860
H	-0.2429700	-2.5104010	-0.0019370
H	-4.7036640	2.6418030	-0.4665970
H	-6.9379800	1.5755520	-0.6598480
H	-7.1205100	-0.9052990	-0.7166140
N	1.0722790	-0.6904750	-2.2795700

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3g¹-PQ-vdW G -1377.730824

C	0.6625470	-0.3124940	1.1844760
C	1.8065380	-0.6728700	0.5652570
C	1.9175980	-2.0387600	-0.0812700
C	0.5723240	-2.4805770	-0.6649010
C	-0.5747020	-2.2706890	0.2952000
C	-0.5175600	-1.1753400	1.1807320
H	2.6733220	-2.0235630	-0.8709280
H	0.5898150	0.6531020	1.6834080
H	2.2432380	-2.7705890	0.6700380
N	2.8515030	0.2416060	0.4544220
H	2.6036940	1.2195630	0.5486720
C	4.2080560	0.0324610	0.2885700
C	4.8389480	-1.2037210	0.5227360
C	6.2088060	1.0218010	-0.2534760
C	6.2065120	-1.2911190	0.3113650
H	4.2812170	-2.0556830	0.8872480
C	6.9204020	-0.1628040	-0.0945040
H	6.7200870	1.9372010	-0.5415530
H	6.7156650	-2.2345240	0.4826650
H	7.9899800	-0.1930800	-0.2637720
C	-1.6054330	-0.9232170	2.0297620
C	-1.7083970	-3.0819490	0.2810530
C	-2.7850860	-2.8253290	1.1307100
H	-3.6641850	-3.4619070	1.1016750
C	-2.7314140	-1.7401270	2.0072920
H	-3.5700730	-1.5254790	2.6630430
H	-1.5639490	-0.0682320	2.7015540
H	-1.7528340	-3.9169310	-0.4143740
H	0.3718260	-1.9097210	-1.5822200
H	0.6294520	-3.5333350	-0.9567390
C	-5.3459080	-0.3353790	-0.2352490
C	-4.2494690	-0.6451410	-1.0292300
C	-3.0813370	0.1176710	-0.9525780
C	-2.9798780	1.2043880	-0.0602720
C	-4.1001540	1.5088240	0.7215820
C	-5.2653640	0.7505440	0.6361590
C	-1.9578500	-0.2453160	-1.8427400
C	-1.7204850	1.9886040	0.0454200
C	-0.6461260	1.7531800	-0.8339620
C	-0.6889700	0.6351160	-1.8006650
C	0.5275730	2.5112060	-0.7672490
H	1.3225960	2.2931820	-1.4743530
C	0.6712920	3.4978250	0.1982230

C	-0.3690330	3.7132780	1.1056740
C	-1.5460430	2.9744690	1.0269130
H	-6.2526430	-0.9277260	-0.2949150
H	-4.2737890	-1.4806880	-1.7215540
H	-4.0831380	2.3476160	1.4067570
H	-6.1162210	1.0138210	1.2566060
H	1.5822430	4.0845770	0.2549570
H	-0.2656890	4.4658790	1.8808110
H	-2.3250670	3.1726600	1.7529810
O	0.2324300	0.3636330	-2.5428880
O	-1.9887770	-1.1766560	-2.6203720
N	4.8900560	1.1285150	-0.0764340

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3g¹-HPQ-vdW G -1377.691611

C	0.8356390	-0.2761790	1.6431530
C	1.9705590	-0.6713860	0.9701000
C	2.0097800	-1.9827340	0.2552560
C	0.6761320	-2.6088190	0.0721700
C	-0.4426880	-2.2023340	0.7503450
C	-0.3743780	-0.9955960	1.5428470
H	2.5070140	-1.8778190	-0.7141820
H	0.8347240	0.6658600	2.1851390
H	2.6198320	-2.6904490	0.8445450
N	3.0582460	0.1488880	0.9872550
H	2.8884400	1.0792460	1.3575720
C	4.2898880	0.0843300	0.3235850
C	4.9512480	-1.1048190	-0.0118250
C	5.9937970	1.3657530	-0.5211460
C	6.1747180	-1.0054510	-0.6636100
H	4.5538890	-2.0740040	0.2517870
C	6.7128890	0.2489580	-0.9385210
H	6.3808400	2.3677000	-0.6857250
H	6.7087260	-1.9091650	-0.9387040
H	7.6650730	0.3626770	-1.4425430
C	-1.5545830	-0.5447110	2.1927890
C	-1.6983020	-2.8973510	0.6444180
C	-2.8038200	-2.4413600	1.2946590
H	-3.7512430	-2.9618440	1.2075690
C	-2.7296750	-1.2399820	2.0662270
H	-3.6270820	-0.8693140	2.5528770
H	-1.5154880	0.3748680	2.7695250
H	-1.7413570	-3.7860030	0.0213820
H	-0.6930930	-1.8502240	-2.3290470
H	0.6357990	-3.5023730	-0.5463060
C	-5.4280810	-0.3629300	-0.9284280
C	-4.1995560	-0.8282170	-1.3457240
C	-3.0198860	-0.0795640	-1.1035980
C	-3.1031080	1.1628020	-0.4103000
C	-4.3786500	1.6081400	-0.0012550
C	-5.5205620	0.8698240	-0.2518270
C	-1.7506870	-0.5682050	-1.5085300
C	-1.8817800	1.9248090	-0.1688210
C	-0.6354170	1.4051050	-0.6020360
C	-0.5492200	0.1061270	-1.2578060
C	0.5493470	2.1394820	-0.3941860
H	1.4785940	1.7122990	-0.7617970
C	0.5235870	3.3579120	0.2559670
C	-0.7043160	3.8736570	0.7105680
C	-1.8775560	3.1727030	0.4950260
H	-6.3241660	-0.9452780	-1.1209030
H	-4.1110770	-1.7782990	-1.8631540
H	-4.4781130	2.5520160	0.5236600
H	-6.4867230	1.2407500	0.0751240
H	1.4416950	3.9169440	0.4120390
H	-0.7362700	4.8299350	1.2235230
H	-2.8085280	3.6038990	0.8466220
O	0.5609990	-0.4541820	-1.5783450
O	-1.6534680	-1.7484330	-2.1809020
N	4.8112350	1.2939290	0.0910290

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3g¹-PQ-TS1 G -1377.676600 ifreq = -1339.32

C	1.0703510	0.1965770	1.5756190
C	2.1637720	-0.3391860	0.9455590
C	2.1543430	-1.7554150	0.4478870
C	0.7817930	-2.3804990	0.3919960
C	-0.2798990	-1.8338840	1.1471150
C	-0.1681150	-0.5025960	1.6658280
H	2.6423250	-1.7968600	-0.5330300
H	1.1124950	1.2181880	1.9460530
H	2.7763830	-2.3618860	1.1255340
N	3.2753720	0.4446970	0.7800830
H	3.1299190	1.4345270	0.9482160
C	4.5096160	0.2169960	0.1706450
C	5.1247570	-1.0385530	0.0434520
C	6.2956260	1.2697280	-0.8188510
C	6.3648520	-1.0970830	-0.5790680
H	4.6761390	-1.9371360	0.4397920
C	6.9710840	0.0720430	-1.0332770
H	6.7329690	2.2152490	-1.1288140
H	6.8596430	-2.0563900	-0.6923790
H	7.9386840	0.0619970	-1.5203200
C	-1.3035160	0.0938060	2.2729080
C	-1.5193690	-2.5227420	1.2995020
C	-2.5941140	-1.9250840	1.9043310
H	-3.5352390	-2.4580910	1.9965330
C	-2.4916310	-0.5905860	2.3790990
H	-3.3555620	-0.1119230	2.8297720
H	-1.2224530	1.1169950	2.6320840
H	-1.6020990	-3.5288930	0.8957090
H	0.1661330	-2.0159850	-0.9398110
H	0.7719830	-3.4579620	0.2315200
C	-4.7510170	-1.9253810	-1.4096740
C	-3.3767180	-1.8815680	-1.5301960
C	-2.6612680	-0.7093280	-1.2073000
C	-3.3520690	0.4402070	-0.7501060
C	-4.7553760	0.3702090	-0.6493710
C	-5.4460800	-0.7866120	-0.9694270
C	-1.2260250	-0.6832610	-1.3515900
C	-2.6011070	1.6618990	-0.4087910
C	-1.2009470	1.7009840	-0.5829360
C	-0.4647160	0.5263250	-1.0901710
C	-0.4662690	2.8421390	-0.2346660
H	0.6088430	2.8211680	-0.3852510
C	-1.1019670	3.9558220	0.2922930
C	-2.4905530	3.9306950	0.4694610
C	-3.2250140	2.8043330	0.1233000
H	-5.2926560	-2.8318590	-1.6606780
H	-2.8177980	-2.7465450	-1.8724920
H	-5.3207550	1.2338740	-0.3189950
H	-6.5276130	-0.8083630	-0.8818620
H	-0.5311450	4.8375850	0.5651410
H	-3.0015240	4.7950620	0.8820070
H	-4.2966870	2.8193910	0.2843680
O	0.7708010	0.5212160	-1.2177260
O	-0.5567440	-1.7284740	-1.7471510
N	5.0979160	1.3490200	-0.2380120

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3g¹PQ-TS2 G -1377.680093 ifreq = -1240.01

C	-1.2533180	0.5035200	-1.3319980
C	-2.4246590	1.3385000	-1.0574420
C	-3.6972070	0.7572720	-0.6991230
C	-3.7720920	-0.6391600	-0.4633250
H	-0.3990210	0.8355370	-0.5960830
H	-0.7317340	0.7227110	-2.2649020
C	1.0181060	-1.5511260	-1.4538310
C	1.9662760	-2.5596500	-1.1784790
C	2.6298800	-0.2003630	-2.3617040
C	3.2815860	-2.3386660	-1.5375050
H	1.6622000	-3.4789090	-0.6876800
C	3.6355080	-1.1292210	-2.1474200

H	2.8526410	0.7607330	-2.8188150
H	4.0320140	-3.0968790	-1.3357080
H	4.6582660	-0.9120540	-2.4316200
C	-5.0075680	-1.2030060	-0.0799460
C	-4.8602050	1.5447590	-0.5605570
C	-6.0626660	0.9712070	-0.1925170
C	-6.1348020	-0.4132700	0.0546640
H	-5.0626280	-2.2726580	0.1044780
H	-1.9649980	1.8379890	0.2044200
H	-2.4539530	2.2981960	-1.5719730
C	-0.8109100	-1.8351840	2.5850050
C	-0.9866470	-0.5478220	2.0944870
C	0.1057690	0.1795830	1.5977900
C	1.4052330	-0.3811330	1.6089250
C	1.5556070	-1.6786730	2.1121340
C	0.4645150	-2.4031870	2.5858980
C	-0.1335430	1.4850200	0.9894630
C	2.5434350	0.3982030	1.0765940
C	2.3344760	1.6667880	0.4930690
C	0.9822670	2.2724590	0.4124840
C	3.4066960	2.4012650	-0.0278410
H	3.1953970	3.3698260	-0.4694090
C	4.6981880	1.8997770	0.0241230
C	4.9194070	0.6486220	0.6073080
C	3.8605010	-0.0875880	1.1222540
H	-1.6620410	-2.3953200	2.9593510
H	-1.9703930	-0.0890330	2.0785430
H	2.5312350	-2.1507970	2.1244250
H	0.6138570	-3.4103260	2.9621180
H	5.5269580	2.4722190	-0.3793250
H	5.9250670	0.2426740	0.6584120
H	4.0719640	-1.0551070	1.5622300
O	0.7759250	3.3586810	-0.1213900
O	-1.2898760	2.0600360	1.1053520
C	-2.5978580	-1.4517770	-0.6242450
C	-1.4015080	-0.9467210	-1.0430320
H	-2.6792550	-2.5134190	-0.3993310
N	-0.3053680	-1.7930370	-1.1068560
H	-0.4689020	-2.7111480	-0.7138300
H	-4.7951230	2.6134700	-0.7478510
H	-6.9507200	1.5867700	-0.0924730
H	-7.0787830	-0.8618420	0.3474550
N	1.3443340	-0.3990970	-2.0353650

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3u¹G -673.330650

C	-1.0189840	-0.1482720	-0.9793790
C	0.1278420	-0.6251240	-0.4426950
C	0.0435120	-1.7526450	0.5653970
C	-1.1045980	-2.7053380	0.2388020
C	-2.3962620	-1.9544090	0.0331370
C	-2.3261710	-0.7013640	-0.6079320
H	0.9799900	-2.3080870	0.6346040
H	-1.0180500	0.7007710	-1.6547930
H	-0.1169590	-1.2933900	1.5518080
C	-3.5136810	-0.0114890	-0.8859770
C	-3.6358210	-2.4757890	0.3962100
C	-4.8141570	-1.7768650	0.1240810
H	-5.7733890	-2.1942680	0.4137500
C	-4.7498320	-0.5432990	-0.5236350
H	-5.6602610	0.0061800	-0.7427030
H	-3.4623150	0.9528450	-1.3855550
H	-3.6805620	-3.4425590	0.8922330
H	-0.8599500	-3.2433760	-0.6890670
H	-1.2174080	-3.4558620	1.0264640
C	2.4574530	-0.9176010	-1.1095890
C	1.4141910	1.2275380	-1.3605120
C	3.8012660	-0.2167840	-0.9949670
H	2.2754470	-1.1856610	-2.1644610
H	2.4852780	-1.8371240	-0.5244580
C	2.7911750	1.8640670	-1.2429780

H	1.1699980	1.0736350	-2.4264120
H	0.6704540	1.9043520	-0.9309740
H	4.5917360	-0.8419040	-1.4154250
H	4.0249150	-0.0155940	0.0638210
H	2.8390400	2.7742340	-1.8442920
H	2.9905260	2.1180810	-0.1908560
N	1.3872120	-0.0339400	-0.6275320
O	3.8059740	0.9990760	-1.7226150

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3u'-PQ-vdW G -1361.855251

C	1.3137300	-0.2431670	0.9410310
C	2.3646620	-0.9612740	0.4802620
C	2.2529970	-2.4711390	0.4054510
C	0.8303070	-2.8996070	0.0399550
C	-0.2135530	-2.2049560	0.8774140
C	0.0440180	-0.8816020	1.2927560
H	2.9462670	-2.8582090	-0.3458950
H	1.3791380	0.8318860	1.0793030
H	2.5421860	-2.9049890	1.3730940
C	-0.9331880	-0.1966190	2.0290680
C	-1.4334150	-2.7994330	1.1910790
C	-2.4067150	-2.1046280	1.9123220
H	-3.3581840	-2.5768860	2.1373900
C	-2.1503680	-0.8001080	2.3348980
H	-2.9028480	-0.2478460	2.8911450
H	-0.7372380	0.8265680	2.3451070
H	-1.6298810	-3.8151680	0.8546750
H	0.6474700	-2.6441220	-1.0135570
H	0.7302090	-3.9853150	0.1316920
C	-4.4194700	-1.8351290	-1.3225600
C	-3.0923220	-1.6303370	-1.6713260
C	-2.4353170	-0.4533640	-1.2990080
C	-3.0938640	0.5387910	-0.5462210
C	-4.4396910	0.3221600	-0.2219690
C	-5.0930570	-0.8448030	-0.6048050
C	-1.0388900	-0.2659030	-1.7498940
C	-2.3671530	1.7520940	-0.0881730
C	-1.0496860	2.0096510	-0.5168440
C	-0.3549930	1.0816010	-1.4370250
C	-0.3448640	3.1273040	-0.0602860
H	0.6688170	3.2806020	-0.4180710
C	-0.9304770	4.0076390	0.8397310
C	-2.2338090	3.7624640	1.2752810
C	-2.9406200	2.6538710	0.8169030
H	-4.9294640	-2.7475720	-1.6124990
H	-2.5392890	-2.3712580	-2.2401360
H	-4.9984460	1.0650510	0.3343340
H	-6.1362440	-0.9815850	-0.3379530
H	-0.3815830	4.8697890	1.2026740
H	-2.7047730	4.4361280	1.9840810
H	-3.9423490	2.4916960	1.1957240
O	0.7176930	1.3277170	-1.9483840
O	-0.4230880	-1.0940750	-2.3898600
C	3.6420950	1.0613880	0.0325410
C	4.7962650	-0.9945380	0.5536450
C	4.8810010	1.5043010	-0.7309030
H	3.6772100	1.4603270	1.0620210
H	2.7544770	1.4595100	-0.4683120
C	5.9898390	-0.4808520	-0.2348070
H	4.9255090	-0.7382540	1.6193010
H	4.7483690	-2.0817710	0.4684280
H	4.9954600	2.5883960	-0.6692280
H	4.7849540	1.2132920	-1.7877690
H	6.9198330	-0.8604110	0.1934550
H	5.9127560	-0.8123540	-1.2815340
N	3.5616070	-0.3941200	0.0392690
O	6.0598490	0.9336700	-0.1871870

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3u'HPQ-vdW G -1361.821072

C	1.2185640	-0.5172200	1.3497520
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C	2.2177270	-1.0773220	0.5538510
C	1.9751000	-2.4149310	-0.0856540
C	0.5736250	-2.9024670	-0.0213880
C	-0.3928850	-2.3027900	0.7278690
C	-0.0655890	-1.0716280	1.4211500
H	2.2788070	-2.3892500	-1.1361490
H	1.3811160	0.4087900	1.8849770
H	2.6208330	-3.1643600	0.4052700
C	-1.0941820	-0.4344960	2.1806350
C	-1.7357020	-2.8262580	0.8213440
C	-2.6791260	-2.1892650	1.5601110
H	-3.6905010	-2.5760450	1.6211810
C	-2.3510560	-0.9663300	2.2385250
H	-3.1260370	-0.4529060	2.8000710
H	-0.8642660	0.5000540	2.6846780
H	-1.9693150	-3.7334610	0.2715250
H	-0.8381460	-1.9718220	-2.3234390
H	0.3508140	-3.8221800	-0.5575030
C	-5.3209540	-0.0863220	-0.6097610
C	-4.1682640	-0.6563490	-1.1045730
C	-2.9193610	0.0060350	-0.9821190
C	-2.8567900	1.2729610	-0.3309490
C	-4.0594030	1.8264900	0.1603290
C	-5.2687160	1.1700550	0.0281800
C	-1.7283230	-0.5881250	-1.4716140
C	-1.5677590	1.9442560	-0.2123790
C	-0.4036880	1.3175850	-0.7277000
C	-0.4658740	0.0057730	-1.3590210
C	0.8487230	1.9545450	-0.6221590
H	1.7066360	1.4338960	-1.0416070
C	0.9707950	3.1848910	-0.0063360
C	-0.1747950	3.8109220	0.5201550
C	-1.4127750	3.2023660	0.4133430
H	-6.2701600	-0.6041580	-0.7111710
H	-4.1932460	-1.6250060	-1.5937290
H	-4.0461010	2.7914200	0.6557630
H	-6.1756670	1.6227660	0.4160250
H	1.9395260	3.6722360	0.0695460
H	-0.0912420	4.7780350	1.0062910
H	-2.2764210	3.7141860	0.8238730
O	0.5710390	-0.6283320	-1.7737400
O	-1.7741190	-1.7950750	-2.1050350
C	3.7866920	0.7618980	1.0264740
C	4.5723850	-1.2015030	-0.1906600
C	4.6807790	1.5979870	0.1189850
H	4.3055050	0.5349900	1.9679000
H	2.8940040	1.3461880	1.2443920
C	5.4089200	-0.2655550	-1.0513700
H	5.1842350	-1.5803340	0.6405090
H	4.2522220	-2.0467810	-0.7955250
H	5.0440130	2.4697760	0.6663030
H	4.1043490	1.9395390	-0.7546310
H	6.3148900	-0.7772470	-1.3808030
H	4.8291710	0.0465650	-1.9328660
N	3.4167140	-0.4910400	0.3640590
O	5.8142760	0.8723010	-0.3149000

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3u'-PQ-TS1 G -1361.804779 ifreq = -1220.90

C	1.4328530	-0.1886540	1.2689430
C	2.3828170	-0.8791910	0.5468870
C	2.1103520	-2.2943390	0.1029960
C	0.6654360	-2.7172790	0.1890770
C	-0.2305110	-2.0171850	1.0228600
C	0.1243740	-0.7080110	1.4878390
H	2.4801630	-2.4230830	-0.9206020
H	1.6343630	0.8070220	1.6458650
H	2.7097960	-2.9766830	0.7282480
C	-0.8502510	0.0488020	2.1937570
C	-1.5330880	-2.5211480	1.3153330
C	-2.4447790	-1.7692010	2.0067530

H	-3.4376710	-2.1599420	2.2064260
C	-2.1042940	-0.4572570	2.4357880
H	-2.8410430	0.1451320	2.9584590
H	-0.5907630	1.0541860	2.5170440
H	-1.7958810	-3.5109950	0.9500930
H	0.0231050	-2.2176960	-1.0736640
H	0.4794310	-3.7795250	0.0351000
C	-4.7855000	-1.6114330	-1.1581290
C	-3.4275200	-1.6751480	-1.3968050
C	-2.5918580	-0.5726950	-1.1184310
C	-3.1467420	0.6175630	-0.5874510
C	-4.5370550	0.6576890	-0.3632340
C	-5.3454130	-0.4322600	-0.6386460
C	-1.1745390	-0.6646090	-1.3819700
C	-2.2733380	1.7705140	-0.3062310
C	-0.8973900	1.7027090	-0.6122740
C	-0.2991480	0.4783570	-1.1864570
C	-0.0497040	2.7833430	-0.3343660
H	0.9996800	2.6858170	-0.5945430
C	-0.5437700	3.9367800	0.2549160
C	-1.9063140	4.0144650	0.5674470
C	-2.7539960	2.9510190	0.2884370
H	-5.4187860	-2.4654880	-1.3768270
H	-2.9731140	-2.5743600	-1.8000890
H	-4.9989620	1.5566010	0.0285240
H	-6.4134380	-0.3698880	-0.4561780
H	0.1162850	4.7705880	0.4716600
H	-2.3078770	4.9102020	1.0309840
H	-3.8012530	3.0451180	0.5513910
O	0.9164090	0.3914940	-1.4247740
O	-0.6416650	-1.7593330	-1.8522130
C	3.8886590	1.0436370	0.5380890
C	4.7749100	-1.1771810	0.0301840
C	4.9444680	1.6016780	-0.4065170
H	4.2318970	1.1162530	1.5819030
H	2.9818670	1.6400130	0.4209270
C	5.7742800	-0.5063030	-0.8990590
H	5.2439360	-1.3392900	1.0131930
H	4.5044390	-2.1476210	-0.3841390
H	5.2541040	2.5937100	-0.0724530
H	4.5228500	1.6792890	-1.4198860
H	6.7003820	-1.0834910	-0.9291090
H	5.3554050	-0.4428150	-1.9145980
N	3.5843630	-0.3402220	0.1938260
O	6.1043690	0.7904040	-0.4371290

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2u'PQ-TS2 G -1361.800546 ifreq = -1371.96

C	1.0492980	-0.4738840	-1.6024900
C	2.2900870	-1.2224350	-1.4572420
C	3.4575260	-0.5898230	-0.8620210
C	3.3451370	0.7299770	-0.3636120
H	0.2523040	-0.9742290	-0.8559810
H	0.5371560	-0.6557440	-2.5488740
C	4.4707210	1.3285870	0.2362390
C	4.6889610	-1.2647610	-0.7640340
C	5.7866000	-0.6566950	-0.1780450
C	5.6738940	0.6483520	0.3300760
H	4.3833790	2.3405260	0.6234870
H	1.8474040	-2.0936710	-0.4555560
H	2.4839130	-1.9871710	-2.2086220
C	0.9738910	0.5308910	3.0845320
C	1.0500500	-0.4691220	2.1229510
C	-0.0991320	-0.8972550	1.4466930
C	-1.3502610	-0.2997290	1.7155110
C	-1.4065200	0.6942300	2.7015710
C	-0.2623960	1.1068670	3.3790860
C	0.0312150	-1.9454830	0.4255630
C	-2.5411070	-0.7138610	0.9421680
C	-2.4444650	-1.7186620	-0.0445520
C	-1.1707550	-2.4443570	-0.2990900

C	-3.5588600	-2.0794170	-0.8119550
H	-3.4351300	-2.8571730	-1.5585190
C	-4.7828190	-1.4569190	-0.6174720
C	-4.8959160	-0.4706520	0.3669440
C	-3.7946210	-0.1079720	1.1320350
H	1.8702620	0.8566740	3.6023790
H	2.0015920	-0.9344350	1.8832640
H	-2.3496410	1.1648390	2.9546050
H	-0.3390040	1.8816090	4.1352120
H	-5.6423750	-1.7346110	-1.2181530
H	-5.8479280	0.0221850	0.5366740
H	-3.9226870	0.6655580	1.8800880
O	-1.0901710	-3.3692940	-1.0969410
O	1.1335900	-2.6132110	0.3268400
C	2.0976270	1.4514080	-0.4821880
C	0.9951620	0.9186180	-1.0801830
H	2.0709200	2.4561540	-0.0736840
H	4.7658650	-2.2765350	-1.1543220
H	6.7305970	-1.1875950	-0.1097570
H	6.5314830	1.1255850	0.7937470
C	-0.4160440	2.7616860	-0.3309870
C	-1.0594400	1.4968480	-2.3017580
C	-1.8939240	3.0544240	-0.1136070
H	0.0599730	3.6053030	-0.8598050
H	0.0600740	2.6467530	0.6481940
C	-2.5081650	1.8350640	-1.9913360
H	-0.6578900	2.2240500	-3.0267090
H	-1.0326670	0.5057870	-2.7561430
H	-2.0173790	4.0316860	0.3577810
H	-2.3241000	2.2814300	0.5406010
H	-3.0820520	1.9114330	-2.9171500
H	-2.9449030	1.0467320	-1.3580510
N	-0.2615800	1.5167230	-1.0716660
O	-2.6087390	3.0877850	-1.3361270

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3m' G -787.631258

C	1.1287930	0.5097500	1.2770050
C	2.1538670	-0.0120220	0.5655630
C	2.0767920	-1.4513950	0.1007930
C	0.6382410	-1.8210360	-0.2640170
C	-0.3240800	-1.4400830	0.8341530
C	-0.0740590	-0.2700960	1.5688080
H	2.7377020	-1.6091440	-0.7555730
H	1.1882150	1.5247700	1.6627280
H	2.4195250	-2.1168380	0.9037830
N	3.2366950	0.7686300	0.1825800
H	3.1012530	1.7684930	0.2508070
C	4.5490050	0.3523330	-0.0661320
C	5.3701600	1.1674330	-0.8618670
C	5.0826930	-0.8256540	0.4747320
C	6.6872830	0.8044040	-1.1185450
H	4.9615350	2.0826870	-1.2812820
C	6.3968280	-1.1929300	0.1890020
H	4.4841100	-1.4393040	1.1377510
C	7.2083980	-0.3857090	-0.6058850
H	7.3062470	1.4498860	-1.7341270
H	6.7915830	-2.1112740	0.6128990
H	8.2330400	-0.6731010	-0.8161310
C	-0.9844120	0.1415060	2.5565030
C	-1.4862230	-2.1796980	1.0917640
C	-2.3861990	-1.7778580	2.0844060
H	-3.2822950	-2.3487070	2.2935410
C	-2.1230480	-0.6118860	2.8077430
H	-0.7881910	1.0480890	3.1217570
H	0.3494650	-1.2968810	-1.1868650
H	0.5738850	-2.8908240	-0.4724450
O	-1.6704590	-3.2844410	0.3113430
C	-2.8249510	-4.0724590	0.5414030
H	-3.7387300	-3.4936270	0.3682330
H	-2.7747760	-4.8946860	-0.1711530

H	-2.8330260	-4.4721700	1.5613850
H	-2.8241410	-0.2962440	3.5744020

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3m'-PQ-vdW G -1476.154947

C	1.3342520	0.5073640	1.2021720
C	2.4012830	-0.0591990	0.5925670
C	2.3409700	-1.5175430	0.1908690
C	0.9360860	-1.8967670	-0.2835400
C	-0.1284580	-1.4152390	0.6710810
C	0.0869670	-0.2258940	1.3922530
H	3.0682560	-1.7236650	-0.5985810
H	1.3816370	1.5354720	1.5538800
H	2.6106350	-2.1426440	1.0521030
N	3.5206370	0.6920190	0.2698640
H	3.3866920	1.6943180	0.2573620
C	4.8347030	0.2511910	0.0861360
C	5.6968860	1.0236470	-0.7084370
C	5.3308840	-0.9100140	0.6951060
C	7.0182160	0.6350050	-0.8974860
H	5.3166610	1.9246540	-1.1819320
C	6.6500480	-1.3037130	0.4772950
H	4.6967030	-1.4898280	1.3557460
C	7.5029420	-0.5388540	-0.3166940
H	7.6691030	1.2469430	-1.5144200
H	7.0155750	-2.2089320	0.9525290
H	8.5310030	-0.8468100	-0.4746520
C	-0.9049540	0.2473750	2.2683850
C	-1.3350300	-2.1144380	0.8475330
C	-2.3073050	-1.6575110	1.7403780
H	-3.2405690	-2.1913190	1.8739200
C	-2.0820860	-0.4671060	2.4373680
H	-0.7422450	1.1784380	2.8052360
H	0.7566170	-1.4617430	-1.2769190
H	0.8693140	-2.9809430	-0.3986770
C	-5.0355530	-1.3043770	-0.9014890
C	-3.7788170	-1.2453020	-1.4861630
C	-2.9376400	-0.1545460	-1.2464940
C	-3.3399710	0.9075890	-0.4134640
C	-4.6155540	0.8302240	0.1629310
C	-5.4488980	-0.2576670	-0.0741830
C	-1.5968010	-0.1706490	-1.8715800
C	-2.4309780	2.0538710	-0.1459470
C	-1.1217710	2.0723500	-0.6668190
C	-0.6247020	0.9726120	-1.5237220
C	-0.2447010	3.1222260	-0.3809340
H	0.7557290	3.0841210	-0.8006890
C	-0.6501590	4.1780540	0.4244980
C	-1.9490560	4.1792700	0.9355670
C	-2.8251750	3.1350090	0.6523840
H	-5.6876600	-2.1527080	-1.0825840
H	-3.4155800	-2.0428710	-2.1270940
H	-4.9728100	1.6146530	0.8188150
H	-6.4281200	-0.2885020	0.3931080
H	0.0303770	4.9924120	0.6490370
H	-2.2861590	5.0000100	1.5608040
H	-3.8229560	3.1768810	1.0713100
O	0.5014490	0.9385710	-1.9768850
O	-1.2325540	-1.0309050	-2.6480270
O	-1.4864990	-3.2318820	0.0813910
C	-2.5965980	-4.0721580	0.3481510
H	-3.5421420	-3.5593550	0.1421340
H	-2.4937730	-4.9265860	-0.3197250
H	-2.5854370	-4.4134770	1.3893620
H	-2.8486590	-0.0977800	3.1127220

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3m'-HPQ-vdW G -1476.124758

C	-0.3881220	0.6587750	-1.6185220
C	-1.4474440	-0.0246330	-1.0649010
C	-1.2877210	-1.4402280	-0.6144160
C	0.0822950	-1.9894940	-0.7503410

C	1.1197650	-1.2678830	-1.2558120
C	0.8954270	0.0837490	-1.7394410
H	-1.5507020	-1.5170350	0.4549470
H	-0.5245320	1.6861720	-1.9490440
H	-2.0218150	-2.0856060	-1.1217270
N	-2.6555240	0.5917850	-0.9420960
H	-2.6974380	1.5149310	-1.3586830
C	-3.9236120	-0.0050780	-0.7077240
C	-4.1844030	-0.7715270	0.4310410
C	-4.9477220	0.2386960	-1.6295700
C	-5.4525620	-1.3168170	0.6225390
H	-3.4117510	-0.9175550	1.1767980
C	-6.2181390	-0.2904990	-1.4184860
H	-4.7413080	0.8375850	-2.5120150
C	-6.4732770	-1.0794830	-0.2968300
H	-5.6446500	-1.9138700	1.5082430
H	-7.0056170	-0.0934290	-2.1386770
H	-7.4611700	-1.4981500	-0.1363930
C	1.9620450	0.7834380	-2.3391790
C	2.4764660	-1.7880160	-1.2756330
C	3.4947980	-1.0618740	-1.8388490
H	4.5117770	-1.4319430	-1.8511490
C	3.2190970	0.2240300	-2.3745670
H	1.7924940	1.7874610	-2.7140580
H	0.2447480	-3.0052400	-0.4061350
C	0.8111340	4.3856590	-0.1426300
C	1.8294200	3.4576570	-0.0437570
C	1.6212330	2.2201130	0.5965280
C	0.3539260	1.9139950	1.1516600
C	-0.6661350	2.8880350	1.0526220
C	-0.4477980	4.0960680	0.4170340
C	2.7364930	1.2696920	0.6652660
C	0.1327320	0.6039340	1.7544480
C	1.2162130	-0.3343840	1.7892030
C	2.4737490	0.0228430	1.2726320
C	0.9880100	-1.6412350	2.3037860
H	1.8096580	-2.3502600	2.2865840
C	-0.2387430	-1.9906520	2.8289820
C	-1.2877450	-1.0513830	2.8506990
C	-1.0933920	0.2186860	2.3213390
H	0.9793450	5.3348990	-0.6421580
H	2.8135540	3.6499170	-0.4600850
H	-1.6486830	2.6904060	1.4681650
H	-1.2517450	4.8231370	0.3522880
H	-0.3959990	-2.9887380	3.2267880
H	-2.2450470	-1.3139920	3.2914010
H	-1.9238730	0.9176880	2.3382640
O	3.5306960	-0.8367550	1.3975690
O	3.8933670	1.5166200	0.2037530
O	2.6108270	-2.9917370	-0.7004690
C	3.9211640	-3.5350170	-0.5951300
H	4.5604210	-2.8648830	-0.0135650
H	3.8081890	-4.4849580	-0.0759510
H	4.3498600	-3.7035600	-1.5880810
H	4.0400960	0.7843300	-2.8098280
H	4.2608320	-0.3678290	0.9499850

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3m'-PQ-TS1 G -1476.107150 ifreq = -1357.67

C	1.2276280	0.4171630	1.6663130
C	2.3129560	-0.1113370	1.0117110
C	2.2672180	-1.4956750	0.4316980
C	0.8730750	-2.0520580	0.2708190
C	-0.1903440	-1.4981090	1.0168800
C	-0.0378580	-0.2337550	1.6753550
H	2.8085730	-1.5053140	-0.5216100
H	1.2988960	1.4073600	2.1101150
H	2.8283290	-2.1694830	1.0968150
N	3.4566210	0.6222910	0.8897420
H	3.3505030	1.6111060	1.0803260
C	4.6436510	0.2653400	0.2092810

C	5.1640510	1.1444650	-0.7466590
C	5.3306660	-0.9146710	0.5115970
C	6.3545290	0.8385680	-1.4010680
H	4.6238310	2.0575940	-0.9798390
C	6.5082970	-1.2247060	-0.1648810
H	4.9583510	-1.5734780	1.2885670
C	7.0263340	-0.3515360	-1.1212000
H	6.7492970	1.5271210	-2.1412690
H	7.0319120	-2.1451730	0.0728910
H	7.9486350	-0.5932100	-1.6388720
C	-1.1562240	0.3504890	2.3191220
C	-1.4784050	-2.1348890	1.0524030
C	-2.5425470	-1.5564690	1.7077570
H	-3.5168170	-2.0291840	1.7230870
C	-2.3713870	-0.2932840	2.3228330
H	-1.0433400	1.3245290	2.7868090
H	0.3632680	-1.6110350	-1.0404260
H	0.8194030	-3.1163600	0.0533160
C	-4.4765980	-1.4684620	-1.7319960
C	-3.0985470	-1.3978820	-1.8046530
C	-2.4135180	-0.2501210	-1.3570430
C	-3.1361290	0.8502410	-0.8331880
C	-4.5393360	0.7543640	-0.7833140
C	-5.2026260	-0.3819620	-1.2189660
C	-0.9713930	-0.2042770	-1.4364040
C	-2.4111680	2.0462600	-0.3661770
C	-1.0047330	2.1060910	-0.4719740
C	-0.2323010	0.9801150	-1.0356730
C	-0.2982010	3.2204110	0.0001170
H	0.7829750	3.2160080	-0.0991570
C	-0.9669310	4.2865100	0.5812320
C	-2.3624530	4.2419740	0.6871870
C	-3.0693320	3.1425050	0.2197190
H	-4.9966770	-2.3568580	-2.0778070
H	-2.5133420	-2.2232830	-2.1978580
H	-5.1283680	1.5791920	-0.3989510
H	-6.2858400	-0.4253360	-1.1674870
H	-0.4171410	5.1466820	0.9496770
H	-2.9001830	5.0698050	1.1389170
H	-4.1478270	3.1405580	0.3275600
O	1.0081410	0.9971190	-1.1040190
O	-0.2837140	-1.2112510	-1.8878080
O	-1.5390950	-3.3074360	0.3800100
C	-2.7413760	-4.0586420	0.4658870
H	-3.5804360	-3.5049860	0.0330620
H	-2.5665150	-4.9683670	-0.1064690
H	-2.9621440	-4.3115840	1.5085290
H	-3.2263450	0.1702240	2.8061260

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3m¹-PQ-TS2 G -1476.100610 ifreq = -1164.72

C	-0.9935420	0.1890650	-1.3379120
C	-2.2790660	0.8138730	-0.9771740
C	-3.4045390	0.0205090	-0.5866310
C	-3.2573800	-1.3800740	-0.4257660
H	-0.1695370	0.6570160	-0.6786450
H	-0.6743980	0.4846990	-2.3411690
C	1.6157750	-1.4958700	-1.5312590
C	2.6499460	-2.3815270	-1.1731900
C	1.9625200	-0.2953930	-2.1670040
C	3.9772180	-2.0804410	-1.4394080
H	2.3976400	-3.3112720	-0.6690860
C	3.3034080	0.0036930	-2.4147470
H	1.2186300	0.4170110	-2.4889670
C	4.3187130	-0.8772120	-2.0614280
H	4.7496090	-2.7856410	-1.1476100
H	3.5429640	0.9471590	-2.8956490
H	5.3568400	-0.6306370	-2.2570030
C	-4.3686990	-2.1523590	-0.0179500
C	-4.6725950	0.6185190	-0.3360160
C	-5.7537100	-0.1539050	0.0517830

H	-6.7220190	0.2919430	0.2409920
C	-5.5855800	-1.5451140	0.2112400
H	-6.4376290	-2.1415730	0.5218820
H	-4.2526510	-3.2245260	0.1084950
H	-1.8427600	1.3783870	0.2994480
H	-2.4877420	1.7765080	-1.4379100
C	-0.1958900	-2.1349080	2.4790860
C	-0.5437890	-0.8654630	2.0379560
C	0.4429990	0.0289300	1.5884020
C	1.8082700	-0.3517470	1.5918110
C	2.1309300	-1.6342250	2.0484940
C	1.1462040	-2.5203830	2.4791160
C	0.0365040	1.3143110	1.0486490
C	2.8282410	0.5956490	1.0992660
C	2.4449460	1.8435920	0.5594840
C	1.0223270	2.2573080	0.4884750
C	3.4063500	2.7362840	0.0697990
H	3.0634360	3.6809660	-0.3397730
C	4.7547620	2.4174060	0.1138600
C	5.1469950	1.1902090	0.6571860
C	4.1999760	0.2968850	1.1394680
H	-0.9653190	-2.8225700	2.8162330
H	-1.5818100	-0.5474730	2.0293660
H	3.1620720	-1.9684800	2.0529630
H	1.4300380	-3.5116660	2.8183190
H	5.4968640	3.1128580	-0.2644700
H	6.1993130	0.9264280	0.7014950
H	4.5423460	-0.6471100	1.5470600
O	0.6689240	3.3205750	-0.0220940
O	-1.1977120	1.7101830	1.1577770
C	-1.9819690	-1.9842730	-0.6705420
C	-0.8904720	-1.2768890	-1.0963670
H	-1.8854710	-3.0532130	-0.4929940
N	0.3134040	-1.9278530	-1.2410410
H	0.2848200	-2.8858160	-0.9136780
O	-4.7073760	1.9635570	-0.5016310
C	-5.9369540	2.6293290	-0.2598720
H	-5.7466520	3.6854740	-0.4426940
H	-6.7154010	2.2707730	-0.9414180
H	-6.2590820	2.4865340	0.7768420

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3l' G -787.631267

C	1.0692650	0.5013690	0.9093240
C	2.2094310	-0.0517080	0.4341500
C	2.2577920	-1.5397730	0.1498130
C	0.9032280	-2.0148910	-0.3786220
C	-0.2231780	-1.5817310	0.5278900
C	-0.1316250	-0.3042780	1.1268730
H	3.0491300	-1.7606650	-0.5713080
H	1.0358000	1.5585880	1.1618280
H	2.4933130	-2.0865120	1.0720950
N	3.3110980	0.7321080	0.1186810
H	3.1342540	1.7246670	0.0396520
C	4.6591290	0.3560340	0.1175320
C	5.5615810	1.1024090	-0.6569600
C	5.1445410	-0.7118880	0.8846200
C	6.9133660	0.7782970	-0.6712650
H	5.1896830	1.9322000	-1.2516880
C	6.4977890	-1.0440850	0.8422770
H	4.4736600	-1.2641860	1.5323950
C	7.3911710	-0.3058430	0.0682410
H	7.5954780	1.3691830	-1.2747880
H	6.8553600	-1.8772520	1.4396080
H	8.4444950	-0.5642170	0.0472520
C	-1.1858210	0.1625030	1.9119560
C	-1.3582480	-2.3476400	0.7466420
C	-2.4184690	-1.8890200	1.5398960
H	-3.2877250	-2.5176300	1.6883430
C	-2.3249070	-0.6229650	2.1191470
H	-1.1362840	1.1409090	2.3818250

H	-1.4340620	-3.3302040	0.2867510
H	0.7439600	-1.5854760	-1.3781960
H	0.9074650	-3.1029690	-0.4915680
O	-3.2902770	-0.0670930	2.9068120
C	-4.4626870	-0.8266040	3.1409760
H	-5.0970240	-0.2138970	3.7800120
H	-4.9868590	-1.0419690	2.2032050
H	-4.2279070	-1.7669580	3.6520110

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3I'-PW-vdW G -1476.155401

C	0.1307630	-0.7114690	0.9205080
C	1.3180280	-1.1490980	0.4314830
C	1.3549410	-2.3642850	-0.4706110
C	0.0917220	-2.4446730	-1.3318570
C	-1.1694820	-2.2519930	-0.5229530
C	-1.1266550	-1.3742390	0.5841780
H	2.2391800	-2.3284540	-1.1125630
H	0.1011290	0.1264570	1.6148430
H	1.4336150	-3.2687100	0.1470720
N	2.4840610	-0.4576740	0.7037480
H	2.3555970	0.4707790	1.0879150
C	3.8125500	-0.8888490	0.6172190
C	4.8152840	0.0808520	0.4551240
C	4.1866330	-2.2345840	0.7379930
C	6.1538140	-0.2890620	0.3956000
H	4.5333340	1.1271450	0.3753070
C	5.5299540	-2.5965260	0.6516200
H	3.4379000	-2.9943300	0.9256850
C	6.5221730	-1.6332320	0.4792090
H	6.9120650	0.4779390	0.2716730
H	5.7992590	-3.6444320	0.7418100
H	7.5660690	-1.9223080	0.4215540
C	-2.2862370	-1.1305680	1.3190340
C	-2.3782500	-2.8445520	-0.8582710
C	-3.5513950	-2.5978750	-0.1323100
H	-4.4759870	-3.0765680	-0.4308000
C	-3.4954390	-1.7330540	0.9617330
H	-2.2726570	-0.4477210	2.1646180
H	-2.4220030	-3.5147710	-1.7138040
H	0.1466370	-1.6704950	-2.1078010
H	0.0649640	-3.4088790	-1.8484230
C	-4.2441300	1.2505040	-0.3780220
C	-3.2450340	0.8741260	-1.2652620
C	-1.9343580	1.3224440	-1.0828160
C	-1.5952920	2.1710520	-0.0092820
C	-2.6156680	2.5284910	0.8803110
C	-3.9200690	2.0741780	0.6995480
C	-0.9020000	0.8368660	-2.0230510
C	-0.2018380	2.6637020	0.1600220
C	0.8379590	2.1785200	-0.6593350
C	0.5718540	1.1687830	-1.7090230
C	2.1530050	2.6260290	-0.5027430
H	2.9127080	2.2247670	-1.1669720
C	2.4660130	3.5603400	0.4769300
C	1.4465380	4.0483030	1.2959910
C	0.1340460	3.6097180	1.1370040
H	-5.2593980	0.8905990	-0.5089380
H	-3.4519680	0.2086340	-2.0974210
H	-2.4062230	3.1605440	1.7349430
H	-4.6858100	2.3613870	1.4131660
H	3.4855960	3.9108310	0.5985360
H	1.6710320	4.7828960	2.0626710
H	-0.6275620	4.0246720	1.7858170
O	1.4491790	0.6261100	-2.3486030
O	-1.1536660	0.1926790	-3.0207240
O	-4.5702080	-1.4085550	1.7381950
C	-5.8236530	-1.9629310	1.3832240
H	-6.5422990	-1.5737310	2.1033780
H	-6.1169720	-1.6589780	0.3715450
H	-5.8037290	-3.0569300	1.4418350

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3I'-HPQ-vdW G -1476.126116

C	0.2736120	1.8885930	0.8076910
C	1.4673160	1.2011730	0.9694600
C	1.5230230	-0.0364020	1.8081310
C	0.1914950	-0.6185690	2.1010480
C	-0.9775520	0.0206140	1.8362490
C	-0.9514070	1.3418410	1.2195140
H	2.1643760	-0.7826360	1.3111650
H	0.2687730	2.8108920	0.2339570
H	2.0039520	0.1609710	2.7791460
N	2.5531670	1.6347900	0.2906670
H	2.2989810	2.0992460	-0.5827910
C	3.8699940	1.1391980	0.3141160
C	4.5681000	1.0940230	-0.9011740
C	4.5103850	0.7589850	1.4973350
C	5.8817660	0.6387810	-0.9312080
H	4.0619710	1.4030050	-1.8130480
C	5.8238400	0.2952660	1.4522820
H	4.0060290	0.8525320	2.4519280
C	6.5141070	0.2271920	0.2432820
H	6.4102660	0.6002470	-1.8782780
H	6.3123100	-0.0001970	2.3753420
H	7.5370140	-0.1327690	0.2172020
C	-2.1719340	1.9980240	0.9833490
C	-2.2544210	-0.5880990	2.1237970
C	-3.4159100	0.0548320	1.8485900
H	-4.3654870	-0.4201700	2.0594590
C	-3.3709010	1.3733580	1.2663260
H	-2.1884220	2.9757320	0.5139550
H	-2.2629190	-1.5830000	2.5595430
H	2.7257480	-0.5186460	-1.4554410
H	0.1767770	-1.5927680	2.5848230
C	-0.2828910	-4.2762610	-0.3122010
C	0.5806330	-3.3027580	-0.1430630
C	0.0819940	-2.1018350	-0.7145040
C	-1.3247530	-1.9110170	-0.8327060
C	-2.1754860	-2.9326800	-0.3599500
C	-1.6769150	-4.0923100	0.2062180
C	0.9682880	-1.0802850	-1.1509670
C	-1.8109040	-0.6645640	-1.4080210
C	-0.8841180	0.3100370	-1.8685890
C	0.5587910	0.1073410	-1.7657830
C	-1.3556380	1.5271700	-2.4043150
H	-0.6146760	2.2475770	-2.7377420
C	-2.7073190	1.7925690	-2.4936430
C	-3.6327100	0.8289850	-2.0499920
C	-3.1898590	-0.3691260	-1.5228620
H	0.1113680	-5.1898630	0.7478910
H	1.6552790	-3.4355430	-0.0692710
H	-3.2518540	-2.8138830	-0.4326780
H	-2.3577860	-4.8597540	0.5602920
H	-3.0570580	2.7358620	-2.9024790
H	-4.6987120	1.0273880	-2.1180750
H	-3.9266710	-1.0908560	-1.1849080
O	1.4262550	0.9651850	-2.1832460
O	2.3167700	-1.2837190	-1.0088600
O	-4.4826060	2.0621040	0.9791270
C	-5.7519450	1.4216530	1.0826820
H	-6.4748180	2.1468510	0.7145200
H	-5.7813420	0.5223690	0.4596360
H	-5.9806940	1.1709420	2.1220430

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3I'-PQ-TS1 G -1476.105549 ifreq = -1380.50

C	1.2100590	0.3496720	1.5601520
C	2.3716410	-0.1603790	1.0386660
C	2.4534590	-1.5825660	0.5605340
C	1.1097410	-2.2320200	0.3308660
C	-0.0422310	-1.6999810	0.9568010
C	-0.0156110	-0.3767080	1.5163590

H	3.0748610	-1.6250910	-0.3414420
H	1.1909280	1.3729930	1.9274920
H	2.9918380	-2.1710370	1.3191530
N	3.4817930	0.6320030	0.9561590
H	3.3000770	1.6228730	1.0579680
C	4.7346020	0.3106620	0.3862670
C	5.2764310	1.1689920	-0.5770340
C	5.4631370	-0.8080680	0.8034470
C	6.5286380	0.9029270	-1.1246420
H	4.7048550	2.0342740	-0.9004410
C	6.7046390	-1.0801990	0.2330220
H	5.0716720	-1.4475390	1.5870780
C	7.2439190	-0.2280170	-0.7304070
H	6.9386740	1.5753220	-1.8713850
H	7.2600410	-1.9535530	0.5598000
H	8.2152640	-0.4395100	-1.1648740
C	-1.2107560	0.1830040	2.0086710
C	-1.2793670	-2.4024320	0.9582870
C	-2.4333500	-1.8465000	1.4460670
H	-3.3601150	-2.4055960	1.4029360
C	-2.4016160	-0.5187570	1.9592260
H	-1.2150120	1.1967190	2.4000330
H	-1.3064280	-3.3992090	0.5246930
H	0.6907210	-1.9010970	-1.0521860
H	1.1376990	-3.3123230	0.1905000
C	-4.0956680	-2.0865290	-2.0726690
C	-2.7225400	-1.9401210	-2.0711890
C	-2.1241430	-0.7361920	-1.6442520
C	-2.9358320	0.3412690	-1.2115770
C	-4.3338870	0.1674980	-1.2340230
C	-4.9089940	-1.0206360	-1.6535170
C	-0.6853380	-0.6105280	-1.6426590
C	-2.3088910	1.5991990	-0.7691790
C	-0.9060400	1.7467550	-0.8276020
C	-0.0405960	0.6402460	-1.2856910
C	-0.2921750	2.9246000	-0.3818990
H	0.7901860	2.9871980	-0.4394810
C	-1.0505320	3.9673350	0.1282300
C	-2.4424630	3.8323510	0.1929360
C	-3.0583900	2.6695720	-0.2499620
H	-4.5447680	-3.0174930	-2.4043510
H	-2.0746140	-2.7488680	-2.3938170
H	-4.9869020	0.9748320	-0.9217270
H	-5.9896230	-1.1231910	-1.6599500
H	-0.5719800	4.8768850	0.4770280
H	-3.0489550	4.6382650	0.5944700
H	-4.1369280	2.5965630	-0.1716290
O	1.1990390	0.7281800	-1.2842090
O	0.0908030	-1.6055720	-1.9691040
O	-3.4991920	0.1203280	2.4278860
C	-4.7447750	-0.5643190	2.3965240
H	-5.4775830	0.1367680	2.7930320
H	-5.0140170	-0.8377120	1.3713180
H	-4.7160590	-1.4587550	3.0275670

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3l'-PQ-TS2 G -1476.098650 ifreq = -1271.02

C	0.6698780	1.1936450	-0.6102140
C	1.8945220	0.8135930	-1.3090570
C	3.1355140	0.6168540	-0.5836830
C	3.1200200	0.6825880	0.8337050
H	-0.1080790	0.2963120	-0.7506140
H	0.0955740	1.9713300	-1.1152270
C	-1.6426910	1.9954780	1.1004460
C	-2.8647230	1.4362550	1.4966740
C	-1.6477370	3.1209720	0.2632970
C	-4.0643610	1.9662180	1.0300670
H	-2.8647020	0.5729740	2.1567560
C	-2.8519120	3.6304090	-0.2154160
H	-0.7125130	3.6121260	0.0134590
C	-4.0670180	3.0553140	0.1585360

H	-5.0007400	1.5101290	1.3369200
H	-2.8380530	4.4962730	-0.8701420
H	-5.0027180	3.4571450	-0.2155290
C	4.3206070	0.4543170	1.5275120
C	4.3374490	0.3473280	-1.2548290
C	5.5128090	0.1352310	-0.5463360
C	5.5053840	0.1825360	0.8614810
H	6.4111990	0.0154760	1.4312340
H	4.3190030	0.4989710	2.6133270
H	1.5156380	-0.5189980	-1.5903840
H	1.9830590	1.1472130	-2.3420580
C	0.3341840	-2.3188530	2.4360080
C	0.5401110	-2.0014910	1.0991560
C	-0.5473120	-1.7301680	0.2574080
C	-1.8704870	-1.7861380	0.7523380
C	-2.0520210	-2.1199170	2.1004470
C	-0.9676800	-2.3751290	2.9363930
C	-0.2858500	-1.3148100	-1.1228150
C	-3.0045350	-1.4620450	-0.1408900
C	-2.7748600	-1.0092070	-1.4573030
C	-1.4062100	-0.9405650	-2.0272070
C	-3.8434110	-0.6423410	-2.2861650
H	-3.6166140	-0.2959560	-3.2891940
C	-5.1500630	-0.7289020	-1.8328640
C	-5.3917910	-1.2027320	-0.5390000
C	-4.3381850	-1.5622920	0.2897940
H	1.1813710	-2.5182140	3.0844810
H	1.5442510	-1.9507930	0.6889360
H	-3.0487520	-2.1700840	2.5236050
H	-1.1425140	-2.6210170	3.9788360
H	-5.9752920	-0.4415490	-2.4757750
H	-6.4104410	-1.2897670	-0.1738670
H	-4.5669570	-1.9213100	1.2863860
O	-1.1850070	-0.5727870	-3.1752890
O	0.8847160	-1.4905520	-1.6474080
C	1.8986180	1.0066330	1.5244860
C	0.7343000	1.2766970	0.8740700
H	1.9161900	1.0351720	2.6119190
N	-0.4449750	1.4556550	1.5894470
H	-0.5117850	0.9349180	2.4548740
O	6.6257460	-0.1145510	-1.2885940
C	7.8468320	-0.3361970	-0.6025340
H	8.5957480	-0.5111090	-1.3733490
H	8.1304420	0.5400060	-0.0095470
H	7.7800460	-1.2149390	0.0479200
H	4.3615550	0.2995310	-2.3398070

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3j' G -787.630896

C	-1.1689520	0.3068650	-1.0795400
C	-2.2439970	-0.1671440	-0.4127370
C	-2.1775160	-1.5402180	0.2273380
C	-0.7722120	-1.7953360	0.7755620
C	0.2830580	-1.5404570	-0.2742550
C	0.0741120	-0.4622610	-1.1638260
H	-2.9195010	-1.6202040	1.0262740
H	-1.2136070	1.2730520	-1.5774500
H	-2.4134330	-2.3125170	-0.5161940
N	-3.3766000	0.6183190	-0.2086530
H	-3.2529540	1.6105240	-0.3596770
C	-4.7018790	0.1837040	-0.1167330
C	-5.6503860	1.0432030	0.4624010
C	-5.1243720	-1.0619110	-0.6019390
C	-6.9822480	0.6591480	0.5621300
H	-5.3286700	2.0104850	0.8387040
C	-6.4582700	-1.4468640	-0.4728920
H	-4.4209660	-1.7167900	-1.1027780
C	-7.3962310	-0.5950580	0.1069280
H	-7.6994590	1.3399170	1.0104220
H	-6.7655840	-2.4172940	-0.8508020
H	-8.4340950	-0.8976620	0.1958500

C	1.0712260	-0.1648830	-2.0933660
C	1.4493170	-2.2855520	-0.3462180
C	2.4379120	-1.9790380	-1.2924620
C	2.2515980	-0.9100570	-2.1691470
H	0.9269150	0.6641530	-2.7816460
H	-0.5916410	-1.1183070	1.6225290
H	-0.6957500	-2.8177750	1.1560530
H	3.0001020	-0.6491030	-2.9074690
H	1.6210840	-3.1163440	0.3331210
O	3.5425010	-2.7786800	-1.2757510
C	4.5663820	-2.5000030	-2.2141310
H	4.9750510	-1.4944440	-2.0642560
H	5.3463650	-3.2396230	-2.0391800
H	4.1959750	-2.5941900	-3.2410170

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3j'-PQ-vdW G -1476.157162

C	-0.5857210	-0.0509580	-1.3389930
C	-1.7585330	-0.5812710	-0.8952970
C	-1.7917660	-2.0178870	-0.4240900
C	-0.4851580	-2.3935050	0.2779210
C	0.7474590	-1.9588560	-0.4776080
C	0.6692290	-0.7903880	-1.2707040
H	-2.6303470	-2.1770170	0.2579400
H	-0.5763800	0.9359840	-1.7947890
H	-1.9500790	-2.6723750	-1.2916160
N	-2.8983960	0.1915840	-0.8456110
H	-2.7364760	1.1916550	-0.7787240
C	-4.2101260	-0.2170160	-0.5728490
C	-5.0249710	0.6170130	0.2063900
C	-4.7466470	-1.3969460	-1.1053370
C	-6.3484120	0.2685860	0.4559680
H	-4.6035920	1.5290060	0.6207870
C	-6.0663170	-1.7478030	-0.8290690
H	-4.1406840	-2.0232940	-1.7513310
C	-6.8756310	-0.9207560	-0.0504170
H	-6.9663670	0.9244310	1.0614050
H	-6.4678880	-2.6670240	-1.2443820
H	-7.9052280	-1.1952400	0.1533070
C	1.8255640	-0.3375450	-1.9073930
C	1.9561480	-2.6201950	-0.3378510
C	3.1139690	-2.1394510	-0.9666090
C	3.0493330	-0.9971120	-1.7639050
H	1.7792360	0.5669850	-2.5103790
H	-0.4709450	-1.9069980	1.2615840
H	-0.4599820	-3.4719420	0.4595410
C	2.1623880	-1.1919960	3.1700830
C	0.9456980	-0.5746750	2.9187120
C	0.8475630	0.4414330	1.9618440
C	1.9868620	0.8869430	1.2603350
C	3.2034370	0.2413420	1.5193430
C	3.2895630	-0.7855690	2.4532960
C	-0.4927580	1.0058820	1.6840190
C	1.8923680	2.0085430	0.2918060
C	0.6503550	2.6047390	-0.0034390
C	-0.5947430	2.1353990	0.6436190
C	0.5540220	3.6548630	-0.9249000
H	-0.4253200	4.0786950	-1.1228680
C	1.6867010	4.1350470	-1.5643790
C	2.9271100	3.5617310	-1.2701620
C	3.0267690	2.5190970	-0.3565930
H	2.2347030	-1.9849020	3.9068300
H	0.0452270	-0.8739840	3.4463870
H	4.1018120	0.5238010	0.9842630
H	4.2457680	-1.2713150	2.6215780
H	1.6117840	4.9477920	-2.2787990
H	3.8247430	3.9303420	-1.7564080
H	4.0068180	2.1025550	-0.1585920
O	-1.6902460	2.6168690	0.4076920
O	-1.5081180	0.6264550	2.2354880
H	3.9274840	-0.6052430	-2.2635130

H	2.0339950	-3.5084150	0.2842610
O	4.2538750	-2.8522880	-0.7318300
C	5.4544740	-2.3697000	-1.3068420
H	5.6824900	-1.3585950	-0.9491350
H	6.2396800	-3.0544500	-0.9893720
H	5.3948620	-2.3637650	-2.4009100

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3j'-PQ-vdW G -1476.116733

C	-1.1796630	-0.1218770	-1.6727250
C	-2.3324000	-0.4919990	-0.9920380
C	-2.3705970	-1.7566160	-0.1984870
C	-1.0412940	-2.3807000	0.0306270
C	0.0969860	-1.9556850	-0.5894780
C	0.0298710	-0.7885860	-1.4533870
H	-2.8811470	-1.5769870	0.7549150
H	-1.1839890	0.7735910	-2.2880540
H	-2.9990040	-2.4897300	-0.7320930
N	-3.4492700	0.2591610	-1.0823450
H	-3.3492600	1.1604600	-1.5345830
C	-4.6577470	0.0453380	-0.3563360
C	-5.0355850	0.9659840	0.6226080
C	-5.4657000	-1.0573650	-0.6382050
C	-6.2256160	0.7785580	1.3229250
H	-4.3899220	1.8124320	0.8365360
C	-6.6448660	-1.2485620	0.0790190
H	-5.1778560	-1.7485190	-1.4244060
C	-7.0277210	-0.3314110	1.0580790
H	-6.5184990	1.4945560	2.0837930
H	-7.2708910	-2.1078360	-0.1383210
H	-7.9500050	-0.4796930	1.6100990
C	1.2409940	-0.3355430	-2.0560870
C	1.3688810	-2.5967500	-0.3772170
C	2.4970550	-2.1273170	-0.9762430
C	2.4299880	-0.9653280	-1.8255580
H	1.2095200	0.5498390	-2.6849540
H	-0.2588530	-1.1210040	2.3430150
H	-1.0117610	-3.2562680	0.6741560
C	4.8150410	-0.3854320	1.8217950
C	3.4777310	-0.6659250	1.9898660
C	2.4821760	0.1767850	1.4289950
C	2.8722710	1.3083520	0.6555690
C	4.2541580	1.5622430	0.5030020
C	5.2101920	0.7448110	1.0752100
C	1.1039690	-0.0960460	1.6222510
C	1.8399730	2.1682180	0.0871350
C	0.4721400	1.8698680	0.3213560
C	0.0754950	0.7055630	1.1057250
C	-0.5335010	2.6938270	-0.2219690
H	-1.5657300	2.4328500	-0.0046510
C	-0.2119030	3.7885090	-1.0010710
C	1.1404180	4.0869230	-1.2493540
C	2.1392550	3.2944510	-0.7120050
H	5.5661460	-1.0364890	2.2594810
H	3.1591370	-1.5357550	2.5555090
H	4.5843360	2.4234290	-0.0678790
H	6.2638720	0.9709850	0.9451160
H	-0.9934890	4.4172810	-1.4171190
H	1.4048010	4.9445540	-1.8603040
H	3.1717640	3.5529620	-0.9204830
O	-1.1458260	0.3719570	1.3094240
O	0.7173260	-1.1622920	2.3726270
H	3.3304740	-0.5764150	-2.2866290
H	1.4290150	-3.4500880	0.2911010
O	3.6616680	-2.7897530	-0.7401220
C	4.8699880	-2.2235990	-1.2267380
H	5.0041950	-1.2026640	-0.8533980
H	5.6689370	-2.8561770	-0.8415890
H	4.8978280	-2.2328580	-2.3218720

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3j'-PQ-TS1 G -1476.103338 ifreq = -1262.22

C	-1.2495560	0.0449990	-1.6066440
C	-2.3866930	-0.4084300	-0.9827110
C	-2.3900770	-1.7133660	-0.2419390
C	-1.0158370	-2.2608760	0.0569890
C	0.0983410	-1.8318380	-0.6990550
C	0.0017800	-0.6115250	-1.4509600
H	-2.9824760	-1.6044620	0.6745420
H	-1.2750310	0.9876620	-2.1487440
H	-2.9266230	-2.4560950	-0.8524460
N	-3.5338160	0.3313900	-1.0388850
H	-3.3999800	1.2905980	-1.3348110
C	-4.7538210	0.0820940	-0.3694310
C	-5.3078600	1.0964100	0.4195410
C	-5.4400320	-1.1269950	-0.5233730
C	-6.5297180	0.8972150	1.0566290
H	-4.7689600	2.0319880	0.5394450
C	-6.6505820	-1.3267560	0.1363820
H	-5.0414930	-1.8967080	-1.1751010
C	-7.2016790	-0.3184450	0.9268590
H	-6.9494340	1.6904970	1.6669100
H	-7.1729980	-2.2702920	0.0144950
H	-8.1490250	-0.4761990	1.4315020
C	1.1837710	-0.0916320	-2.0384740
C	1.3509540	-2.4940460	-0.6189120
C	2.4743890	-1.9642960	-1.2090800
C	2.3946300	-0.7291950	-1.9169480
H	1.1248050	0.8499040	-2.5791430
H	-0.5429010	-1.5838980	1.3079010
H	-0.9971080	-3.2836650	0.4313000
C	4.2572670	-1.2445820	2.1658100
C	2.8779140	-1.2059670	2.1458550
C	2.1930630	-0.1242220	1.5520990
C	2.9242320	0.9335140	0.9570410
C	4.3311520	0.8771900	1.0089360
C	4.9900520	-0.1879270	1.5999370
C	0.7495440	-0.1005960	1.5618530
C	2.2066340	2.0511170	0.3192690
C	0.7956700	2.0881990	0.3468460
C	0.0150260	1.0159610	0.9993860
C	0.0960400	3.1254890	-0.2841320
H	-0.9885390	3.1098540	-0.2375760
C	0.7760920	4.1333730	-0.9507360
C	2.1753560	4.1077800	-0.9853610
C	2.8756800	3.0848670	-0.3599580
H	4.7733240	-2.0837530	2.6214550
H	2.2900700	-2.0073490	2.5814220
H	4.9238220	1.6787170	0.5828830
H	6.0752780	-0.2033720	1.6224760
H	0.2310840	4.9334190	-1.4414730
H	2.7211680	4.8891970	-1.5048860
H	3.9580980	3.0929380	-0.4162630
O	-1.2285900	1.0168080	1.0038410
O	0.0581490	-1.0635670	2.1060100
H	3.2768700	-0.2884340	-2.3655180
H	1.4382510	-3.4131180	-0.0462520
O	3.6300100	-2.6639300	-1.0710290
C	4.8270670	-2.0882470	-1.5720440
H	5.0156630	-1.1139600	-1.1085250
H	5.6246530	-2.7791950	-1.3022270
H	4.7888560	-1.9840900	-2.6617980

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3jⁱ-PQ-TS2 G -1476.100165 -ifreq = -1255.54

C	-0.6176920	1.3716410	0.6010140
C	-1.7641690	1.0970170	1.4725530
C	-3.0616230	0.7832320	0.9192170
C	-3.2020770	0.6288590	-0.4863870
H	0.1949000	0.5475000	0.8047200
H	-0.0528510	2.2538120	0.9039330
C	1.5210370	1.8085410	-1.4210810
C	2.6429290	1.1149570	-1.8907110

C	1.7029590	3.0078640	-0.7187100
C	3.9242220	1.5904930	-1.6251160
H	2.5015970	0.1923260	-2.4470660
C	2.9883730	3.4615120	-0.4341350
H	0.8421610	3.6000030	-0.4262790
C	4.1059400	2.7549170	-0.8797320
H	4.7834350	1.0335560	-1.9857690
H	3.1138890	4.3859900	0.1207650
H	5.1055680	3.1138460	-0.6582280
C	-4.4535040	0.2835090	-1.0180850
C	-4.1926340	0.6044520	1.7357530
C	-5.4278420	0.2736030	1.2053720
C	-5.5544230	0.1055650	-0.1887040
H	-4.5802520	0.1589840	-2.0895240
H	-1.3153010	-0.1645670	1.9370800
H	-1.7531170	1.5878360	2.4450820
C	-0.6012070	-2.6343710	-1.7892920
C	-0.6480470	-2.0786950	-0.5175870
C	0.5329760	-1.6961000	0.1364810
C	1.7889470	-1.8795570	-0.4877310
C	1.8095050	-2.4530370	-1.7656950
C	0.6336140	-2.8205480	-2.4143140
C	0.4417250	-1.0537970	1.4450610
C	3.0204860	-1.4416510	0.2030220
C	2.9456880	-0.7466320	1.4290620
C	1.6504010	-0.5272970	2.1205300
C	4.1066950	-0.2751340	2.0565110
H	3.9989330	0.2578600	2.9956030
C	5.3533590	-0.4958650	1.4930980
C	5.4418670	-1.2093350	0.2928050
C	4.2962820	-1.6722800	-0.3389980
H	-1.5200090	-2.9191920	-2.2921380
H	-1.5981150	-1.9278800	-0.0136240
H	2.7504470	-2.6068050	-2.2817330
H	0.6834360	-3.2540870	-3.4079490
H	6.2500780	-0.1290370	1.9813820
H	6.4123000	-1.4034860	-0.1535710
H	4.4056500	-2.2178550	-1.2690410
O	1.5653380	0.0683940	3.1912070
O	-0.6643030	-1.0970280	2.1183950
C	-2.0664020	0.8485330	-1.3427170
C	-0.8450820	1.2206540	-0.8650810
H	-2.1969720	0.7086070	-2.4134040
N	0.2372160	1.3160050	-1.7194140
H	0.1568060	0.7915040	-2.5810440
H	-4.0897260	0.7272710	2.8108060
O	-6.7199570	-0.2247740	-0.8042790
C	-7.8715850	-0.4149700	0.0025630
H	-8.1286190	0.5015230	0.5441050
H	-8.6778210	-0.6701770	-0.6832510
H	-7.7229130	-1.2343130	0.7137040
H	-6.2769430	0.1455220	1.8649570

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CQ G -1070.743421

C	-1.0059660	2.5129900	-1.3528180
C	-1.5826420	1.2693530	-1.5051720
C	-0.8078740	0.1054140	-1.3722110
C	0.5611090	0.1805910	-1.0836980
C	1.1582760	1.4579860	-0.9260090
C	0.3680120	2.6313080	-1.0621040
C	-1.4623270	-1.2084330	-1.5427840
C	1.3844700	-1.0202330	-0.9409440
C	0.8450220	-2.3051360	-1.0859280
C	-0.5903140	-2.4806450	-1.3902130
C	1.6512380	-3.4466570	-0.9457310
H	1.1915280	-4.4219790	-1.0661160
C	2.9951490	-3.3215390	-0.6617600
C	3.5760880	-2.0466490	-0.5084630
C	2.7665880	-0.8870480	-0.6489900
H	-1.6042370	3.4133430	-1.4553460

H	-2.6389880	1.1642400	-1.7291430
H	3.6191800	-4.2035230	-0.5532980
O	-1.1162320	-3.5653310	-1.5257230
O	-2.6416960	-1.3390730	-1.7948010
C	2.5551070	1.5774830	-0.6311980
C	3.3562480	0.4091640	-0.4925940
C	0.9901690	3.9152690	-0.8993610
C	4.9727430	-1.8918690	-0.2126230
H	5.5800290	-2.7860150	-0.1080780
C	4.7308330	0.5307020	-0.2023090
C	3.1390280	2.8517110	-0.4766070
C	2.3164180	4.0197180	-0.6192060
C	4.5229420	2.9494190	-0.1847110
C	5.2960840	1.8221010	-0.0514780
H	6.3555600	1.9072180	0.1722120
C	5.5244500	-0.6579620	-0.0662540
H	0.3749270	4.8037500	-1.0056670
H	2.7784290	4.9953810	-0.4978290
H	4.9651690	3.9345200	-0.0673040
H	6.5820440	-0.5506500	0.1575400

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3a¹-CQ-vdW G-1743.892702

C	1.4949930	0.3340000	1.3330240
C	2.7444520	-0.1411070	1.0610390
C	3.0201750	-1.6213790	1.1931910
C	1.7929990	-2.4424880	0.7935570
C	0.5095390	-1.9389070	1.4088150
C	0.3884570	-0.5554270	1.6607750
H	3.8710050	-1.9087570	0.5710220
H	1.3209970	1.4065120	1.3713500
H	3.2918300	-1.8362110	2.2354920
N	3.7406150	0.7136830	0.6562380
H	3.4205390	1.5926230	0.2620760
C	5.0995850	0.4327070	0.4449210
C	5.7377940	1.0147560	-0.6590250
C	5.8431350	-0.3526200	1.3347750
C	7.0959440	0.8026310	-0.8734410
H	5.1532550	1.6190840	-1.3475280
C	7.1973670	-0.5781640	1.0971020
H	5.3694910	-0.7644620	2.2194530
C	7.8323370	-0.0033600	-0.0035600
H	7.5770850	1.2590550	-1.7328550
H	7.7620470	-1.1925180	1.7915410
H	8.8892600	-0.1753230	-0.1776240
C	-0.8225310	-0.0571960	2.1637640
C	-0.5738420	-2.7785290	1.6511930
C	-1.7812900	-2.2727610	2.1420300
H	-2.6219740	-2.9388130	2.3118190
C	-1.9003200	-0.9079280	2.4016640
H	-2.8375490	-0.5022050	2.7735290
H	-0.9186510	1.0107890	2.3501200
H	-0.4784380	-3.8413380	1.4384980
H	1.6940250	-2.3986950	-0.2983850
H	1.9527870	-3.4931810	1.0534170
C	-1.0380100	-2.8334600	-2.0577540
C	0.0680750	-2.0243630	-2.2023190
C	0.0416070	-0.6910450	-1.7579800
C	-1.1249570	-0.1457410	-1.2057030
C	-2.2702330	-0.9713540	-1.0640270
C	-2.2185900	-2.3295410	-1.4735750
C	1.2749750	0.1161960	-1.8492980
C	-1.1883790	1.2476470	-0.7722960
C	-0.0765110	2.0943050	-0.8599800
C	1.2133930	1.5788280	-1.3613330
C	-0.1543110	3.4336620	-0.4383980
H	0.7314540	4.0547760	-0.5226430
C	-1.3303360	3.9362400	0.0754500
C	-2.4690110	3.1111330	0.1935770
C	-2.3990200	1.7591700	-0.2344520
H	-1.0100850	-3.8683540	-2.3861340

H	0.9846850	-2.4033270	-2.6436050
H	-1.3906540	4.9700470	0.4026750
O	2.2271280	2.2557250	-1.4099380
O	2.3269060	-0.3096140	-2.2883440
C	-3.4760800	-0.4513820	-0.4937150
C	-4.5956420	-1.2906490	-0.3200700
C	-3.5424840	0.9107260	-0.0858740
C	-5.7767800	-0.7611500	0.2603450
C	-4.7285330	1.4166780	0.4855830
C	-5.8422730	0.5536450	0.6503750
H	-6.6336960	-1.4157060	0.3925380
H	-6.7512300	0.9503550	1.0936170
C	-3.6953940	3.6044770	0.7524410
C	-4.7766540	2.7914300	0.8941680
C	-3.3729340	-3.1606000	-1.2849600
C	-4.5104590	-2.6629550	-0.7291210
H	-3.7384870	4.6428150	1.0679270
H	-5.6988290	3.1710750	1.3252050
H	-5.3791430	-3.3000430	-0.5875500
H	-3.3178090	-4.1996010	-1.5968090

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3a¹ HCQ-vdW G-1743.860158

C	2.0854790	0.2861750	1.6195750
C	3.3445950	0.0856010	1.0639900
C	3.8386930	-1.2945730	0.7756660
C	2.7955990	-2.3479830	0.8578590
C	1.5431090	-2.1174610	1.3392890
C	1.1702730	-0.7637370	1.7249400
H	4.3246010	-1.3152690	-0.2065150
H	1.7632390	1.2935830	1.8676300
H	4.6320630	-1.5460500	1.4999100
N	4.1589420	1.1268050	0.8198310
H	3.7705110	2.0542690	0.9473940
C	5.4451730	1.0424530	0.2029380
C	5.6059080	1.4922350	-1.1078000
C	6.5282110	0.5270080	0.9155060
C	6.8623620	1.4250140	-1.7074700
H	4.7471640	1.8786790	-1.6482480
C	7.7780130	0.4486690	0.3044380
H	6.3897450	0.2035610	1.9428950
C	7.9466420	0.8989410	-1.0052940
H	6.9898590	1.7747790	-2.7265940
H	8.6213770	0.0465090	0.8561040
H	8.9222430	0.8420360	-1.4768200
C	-0.1627400	-0.5390400	2.1868090
C	0.5563040	-3.1703830	1.4385570
C	-0.6962450	-2.9076120	1.8870850
H	-1.4409060	-3.6939830	1.9454380
C	-1.0611990	-1.5652250	2.2513390
H	-2.0780840	-1.3678190	2.5782600
H	-0.4578150	0.4735160	2.4482680
H	0.8444140	-4.1697420	1.1249720
H	1.8190700	-2.4069130	-1.7778910
H	3.0866590	-3.3550060	0.5688070
C	-3.2554240	-3.1661190	-1.1053370
C	-1.9114380	-3.0706220	-1.3337950
C	-1.2306480	-1.8190010	-1.2043030
C	-1.9751270	-0.6678290	-0.8315580
C	-3.3756120	-0.7760490	-0.5942240
C	-4.0285950	-2.0246990	-0.7269560
C	0.1556150	-1.6922620	-1.3913350
C	-1.3197790	0.5913550	-0.7004470
C	0.0734440	0.7008920	-0.9138090
C	0.8552980	-0.4675060	-1.2511560
C	0.7034260	1.9642690	-0.7622560
H	1.7738820	2.0171700	-0.9434120
C	-0.0131740	3.0752960	-0.3978750
C	-1.4167390	2.9939440	-0.1601250
C	-2.0658080	1.7446330	-0.3129150
H	-3.7601570	-4.1236520	-1.2064190

H	-1.3342260	-3.9471380	-1.6112720
H	0.4788310	4.0382560	-0.2859220
O	2.1303060	-0.4670320	-1.3847020
O	0.9131780	-2.7718050	-1.7226540
C	-4.1259330	0.3779310	-0.2098970
C	-5.5156440	0.2710290	0.0337720
C	-3.4703620	1.6387920	-0.0685230
C	-6.2383570	1.4395750	0.4182920
C	-4.2099300	2.7810850	0.3168570
C	-5.6098610	2.6474000	0.5548500
H	-7.3058000	1.3531780	0.6032540
H	-6.1738120	3.5285310	0.8493330
C	-2.1876440	4.1292260	0.2264590
C	-3.5339320	4.0279020	0.4557670
C	-5.4267920	-2.1035750	-0.4788630
C	-6.1480300	-0.9966050	-0.1109650
H	-1.6838210	5.0859510	0.3372270
H	-4.1083280	4.9024120	0.7495740
H	-7.2157260	-1.0724150	0.0757410
H	-5.9202440	-3.0662480	-0.5861890

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3a¹-CQ-TS1 G -1743.839780 ifreq = -1448.14

C	2.3413310	0.4942920	1.5649120
C	3.5504760	0.1079100	1.0346680
C	3.8542050	-1.3400220	0.7781150
C	2.6334090	-2.2290690	0.7546980
C	1.4446800	-1.8090380	1.4005680
C	1.2704160	-0.4239270	1.7354610
H	4.4290470	-1.4294650	-0.1509800
H	2.1577420	1.5469410	1.7678440
H	4.5225920	-1.6991980	1.5756230
N	4.4933160	1.0462830	0.7417270
H	4.1517570	1.9992820	0.7138140
C	5.7579290	0.8419520	0.1410750
C	6.0912920	1.5845480	-0.9965580
C	6.6918520	-0.0411280	0.6916870
C	7.3448080	1.4346990	-1.5839810
H	5.3593270	2.2657380	-1.4208710
C	7.9350980	-0.2022600	0.0842550
H	6.4557070	-0.5797960	1.6030580
C	8.2679850	0.5337760	-1.0527620
H	7.5939920	2.0146920	-2.4667620
H	8.6524420	-0.8932710	0.5153350
H	9.2408390	0.4110510	-1.5169860
C	0.0075630	0.0035020	2.2270540
C	0.3600300	-2.7084820	1.6215160
C	-0.8411360	-2.2658680	2.1097480
H	-1.6633830	-2.9601240	2.2524390
C	-1.0260300	-0.8860430	2.3959690
H	-1.9902960	-0.5359380	2.7524350
H	-0.1346300	1.0598830	2.4421800
H	0.4985580	-3.7550890	1.3613110
H	2.0886000	-2.1630720	-0.5952990
H	2.8447850	-3.2981740	0.7671680
C	-2.6147510	-3.3277880	-1.1890870
C	-1.3024500	-2.9586270	-1.3381550
C	-0.9026420	-1.6083640	-1.1630180
C	-1.8670000	-0.6347080	-0.8379750
C	-3.2283080	-1.0190030	-0.6783690
C	-3.6098720	-2.3711580	-0.8536950
C	0.4769590	-1.2257870	-1.2887900
C	-1.4874310	0.7493770	-0.6646690
C	-0.1533960	1.1548980	-0.8163020
C	0.8878010	0.1700230	-1.1478130
C	0.2075860	2.5008710	-0.6028760
H	1.2505820	2.7758370	-0.7254050
C	-0.7393090	3.4341930	-0.2436500
C	-2.0959470	3.0609100	-0.0856210
C	-2.4698250	1.7092990	-0.2960760
H	-2.9112930	-4.3642810	-1.3257020

H	-0.5420740	-3.6919680	-1.5865640
H	-0.4575760	4.4705040	-0.0784520
O	2.0896130	0.4760850	-1.2287130
O	1.4111210	-2.0993250	-1.5235600
C	-4.2145140	-0.0457530	-0.3224660
C	-5.5624810	-0.4327910	-0.1534970
C	-3.8354010	1.3153410	-0.1264510
C	-6.5234520	0.5512310	0.2090810
C	-4.8068790	2.2718940	0.2386590
C	-6.1579760	1.8587190	0.3995920
H	-7.5587930	0.2471410	0.3361310
H	-6.9008680	2.6008400	0.6787310
C	-3.1032170	4.0095840	0.2838710
C	-4.4041220	3.6309320	0.4381000
C	-4.9813000	-2.7344820	-0.6840540
C	-5.9215960	-1.8031990	-0.3474560
H	-2.8081050	5.0434810	0.4399950
H	-5.1598200	4.3597530	0.7181200
H	-6.9612370	-2.0913970	-0.2189940
H	-5.2632730	-3.7741660	-0.8263320

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3a¹-CQ-TS2 G -1743.837947 ifreq = -1187.21

C	-2.6101440	-1.1965500	0.9653880
C	-3.8843930	-1.4579550	0.2878970
C	-4.9239900	-0.4591170	0.2305010
C	-4.6493370	0.8437890	0.7185820
H	-1.7530060	-1.3320970	0.1535840
H	-2.3455080	-1.9841080	1.6707700
C	0.0481360	-0.0825960	2.1806120
C	1.1734010	0.7537520	2.3053480
C	0.2357070	-1.4676250	2.2957790
C	2.4361240	0.2290610	2.5406400
H	1.0479380	1.8293550	2.1985480
C	1.5138940	-1.9844930	2.5128120
H	-0.5887000	-2.1621700	2.2383900
C	2.6207180	-1.1512440	2.6414080
H	3.2842160	0.9039040	2.6180550
H	1.6319920	-3.0614860	2.5843790
H	3.6102320	-1.5660620	2.8034170
C	-5.6533020	1.8330990	0.6249210
C	-6.1940280	-0.7416860	-0.3175460
C	-7.1647000	0.2383520	-0.3905740
H	-8.1385020	0.0098220	-0.8111510
C	-6.8882920	1.5378670	0.0797330
H	-7.6504380	2.3081320	0.0170530
H	-5.4414230	2.8330230	0.9941160
H	-6.3956390	-1.7449430	-0.6839750
H	-3.3795680	-1.4118760	-1.0316120
H	-4.2036090	-2.4991790	0.2686430
C	-1.0063860	2.4984070	-1.3432600
C	-1.5771330	1.2532740	-1.5119090
C	-0.7919710	0.0874210	-1.4003540
C	0.5825880	0.1848660	-1.1252480
C	1.1722350	1.4630230	-0.9689950
C	0.3704390	2.6310140	-1.0653060
C	-1.4152710	-1.2256330	-1.4987390
C	1.3920670	-1.0099830	-0.9787380
C	0.8322900	-2.2929220	-1.0870880
C	-0.6071670	-2.4693990	-1.3651690
C	1.6360160	-3.4365350	-0.9231710
H	1.1658860	-4.4103630	-1.0141190
C	2.9808900	-3.3169930	-0.6498780
C	3.5768790	-2.0422380	-0.5277540
C	2.7794120	-0.8818020	-0.6980570
H	-1.6171780	3.3937150	-1.4219240
H	-2.6362370	1.1528620	-1.7279640
H	3.5973060	-4.2017740	-0.5184640
O	-1.1415940	-3.5735290	-1.4433230
O	-2.6376530	-1.3376630	-1.9164350
C	-3.3720760	1.1303980	1.3045540

C	-2.3923680	0.1878890	1.4580060
H	-3.1879070	2.1466560	1.6473320
N	-1.1802320	0.5689710	1.9952700
H	-1.1109050	1.5699590	2.1311190
C	2.5696600	1.5829680	-0.6820170
C	3.3712050	0.4131450	-0.5525210
C	0.9848810	3.9135170	-0.8739210
C	4.9688590	-1.8909770	-0.2185510
H	5.5707180	-2.7865490	-0.0924810
C	4.7408850	0.5323920	-0.2352360
C	3.1443730	2.8567270	-0.4883040
C	2.3134440	4.0220530	-0.5971340
C	4.5265860	2.9518200	-0.1800330
C	5.3009400	1.8242910	-0.0588460
H	6.3569250	1.9080720	0.1828170
C	5.5259810	-0.6564250	-0.0775500
H	0.3635330	4.8012260	-0.9537390
H	2.7682480	4.9978350	-0.4508430
H	4.9643770	3.9356500	-0.0357150
H	6.5805290	-0.5525740	0.1632510

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H2CQ' G -1071.953394

H	1.9912990	2.6136810	-0.0171820
C	3.4304490	-1.1882000	-0.0068220
C	2.7799730	-0.0027490	-0.2242690
C	1.3561460	0.0589560	-0.2210190
C	0.6157100	-1.1268760	-0.0064110
C	1.2989560	-2.3591760	0.2128580
C	2.7117120	-2.3957090	0.2238600
C	0.6427040	1.2736230	-0.4187540
C	-0.8103240	-1.0959340	-0.0331460
C	-1.4953630	0.1177120	-0.2580830
C	-0.7307970	1.3043990	-0.4471180
C	-2.9187830	0.1314780	-0.2774750
H	-3.4294050	1.0720050	-0.4530510
C	-3.6276720	-1.0225390	-0.0757860
C	-2.9678390	-2.2640570	0.1570290
C	-1.5550880	-2.2942790	0.1801380
H	4.5163620	-1.2215270	-0.0155840
H	3.3576390	0.8950730	-0.4204120
H	-4.7138780	-1.0053000	-0.0914580
O	-1.3983940	2.4690630	-0.6460790
O	1.2794730	2.4717740	-0.6550700
C	-0.8717840	-3.5268200	0.4081580
C	0.5547810	-3.5586740	0.4293210
C	-1.6084460	-4.7141210	0.6187350
C	1.2313760	-4.7789530	0.6527220
C	-0.9028090	-5.9315700	0.8464720
C	0.4655910	-5.9628840	0.8629950
H	-1.4737280	-6.8418550	1.0075270
H	0.9903930	-6.8982220	1.0367340
C	-3.6878060	-3.4763350	0.3705790
C	-3.0329190	-4.6571060	0.5932200
C	3.3707410	-3.6391030	0.4530920
C	2.6574520	-4.7880770	0.6615960
H	4.4570890	-3.6588160	0.4592670
H	3.1713350	-5.7293680	0.8353630
H	-3.5937190	-5.5735860	0.7544870
H	-4.7737330	-3.4461910	0.3528810
H	-0.7441500	3.1788240	-0.7365300

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H2CQ' G -1071.932168

H	0.6004950	1.6420700	1.0620830
H	0.8248200	3.0149790	-1.0152890
C	3.4716450	-1.2349860	0.0530240
C	2.8256710	-0.0158580	-0.0611820
C	1.4270780	0.0499750	-0.0284770
C	0.6684470	-1.1148090	0.1002970
C	1.3237520	-2.3647050	0.2472250
C	2.7405190	-2.4252650	0.2275710

C	0.7268480	1.3838670	-0.0102000
C	-0.7901570	-1.0681290	0.0614340
C	-1.4791760	0.1206900	-0.2150740
C	-0.7070520	1.3402070	-0.5108150
C	-2.8829700	0.1424950	-0.2938550
H	-3.3747560	1.0819130	-0.5251140
C	-3.6098530	-1.0059250	-0.0653590
C	-2.9527140	-2.2278740	0.2002760
C	-1.5341550	-2.2636070	0.2450860
H	4.5565590	-1.2815870	0.0226080
H	3.3925430	0.9016670	-0.1772480
H	-4.6950650	-0.9873370	-0.0997620
O	-1.1702030	2.3199740	-1.0727700
O	1.4674100	2.3809190	-0.6576400
C	-0.8599040	-3.5115060	0.4460460
C	0.5641440	-3.5642160	0.4336980
C	-1.6055310	-4.6938220	0.6327940
C	1.2243050	-4.7993130	0.6014520
C	-0.9196630	-5.9228530	0.8133490
C	0.4522240	-5.9741430	0.7961610
H	-1.5000950	-6.8293150	0.9600480
H	0.9664440	-6.9216800	0.9298800
C	-3.6844670	-3.4440970	0.4093630
C	-3.0379710	-4.6231600	0.6205000
C	3.3854010	-3.6989960	0.3887910
C	2.6595990	-4.8345880	0.5715060
H	4.4709270	-3.7346610	0.3664370
H	3.1564590	-5.7923260	0.6976460
H	-3.6019730	-5.5392400	0.7729360
H	-4.7695600	-3.4048010	0.3878330

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H2O-2*aniso G -769.629788

O	1.48620	2.96564	-0.13358
O	1.98166	0.31639	-1.11853
H	1.69207	2.12267	-0.56958
H	0.63723	2.79776	0.30176
C	3.35899	0.09727	-1.43384
H	3.63301	0.84513	-2.17795
H	3.97996	0.21693	-0.53959
H	3.49722	-0.90691	-1.84737
C	1.48637	-0.57378	-0.18187
C	1.57126	-0.26366	1.17420
C	0.89069	-1.75602	-0.61318
C	1.05789	-1.16131	2.11034
H	2.02822	0.67406	1.47935
C	0.37824	-2.64445	0.33001
H	0.82054	-1.95635	-1.67797
C	0.46326	-2.35205	1.69157
H	1.12288	-0.92796	3.16905
H	-0.09868	-3.56186	-0.00117
H	0.06187	-3.04596	2.42323
O	-1.00558	1.89844	0.88616
C	-1.24769	1.76022	2.27879
H	-0.79925	0.83755	2.66136
H	-0.77744	2.62124	2.75211
H	-2.32273	1.76707	2.48656
C	-1.49276	0.93149	0.05060
C	-1.25212	1.12731	-1.31452
C	-2.19219	-0.19267	0.48916
C	-1.71486	0.19745	-2.23611
H	-0.69927	2.00707	-1.63007
C	-2.65251	-1.11691	-0.45250
H	-2.37515	-0.36494	1.54301
C	-2.42151	-0.93195	-1.81138
H	-1.52224	0.35518	-3.29292
H	-3.19227	-1.99337	-0.10634
H	-2.78257	-1.65684	-2.53344

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2*aniso G -693.214470

O	-2.3537290	-2.4752570	-0.2981850
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C	-1.2999810	-1.8436690	-1.0030590
H	-1.2746720	-2.3086270	-1.9878710
H	-1.4872470	-0.7696310	-1.1095630
H	-0.3399960	-2.0009580	-0.4981950
C	-2.5987270	-2.0625710	0.9751420
C	-1.8890550	-1.0468250	1.6208330
C	-3.6292530	-2.7327810	1.6464870
C	-2.2239470	-0.7067500	2.9336220
H	-1.0970860	-0.5072270	1.1151410
C	-3.9477400	-2.3855110	2.9521470
H	-4.1685290	-3.5144070	1.1206650
C	-3.2476480	-1.3669580	3.6065050
H	-1.6742360	0.0913090	3.4246590
H	-4.7503920	-2.9095970	3.4624480
H	-3.4987960	-1.0959140	4.6271240
O	-3.5760200	2.0418350	1.5220110
C	-4.0960780	2.3148660	2.8121350
H	-4.0986020	1.4122850	3.4328830
H	-3.4344340	3.0599230	3.2523790
H	-5.1124760	2.7193740	2.7465240
C	-4.2399010	1.1339610	0.7545880
C	-3.7288620	0.9370740	-0.5354470
C	-5.3577840	0.4156310	1.1804600
C	-4.3277680	0.0185760	-1.3863880
H	-2.8582760	1.5100020	-0.8408880
C	-5.9487520	-0.5055120	0.3105690
H	-5.7613590	0.5452060	2.1774370
C	-5.4449220	-0.7119260	-0.9686330
H	-3.9181850	-0.1337490	-2.3809160
H	-6.8104540	-1.0710800	0.6529910
H	-5.9081600	-1.4341240	-1.6326290

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PhOH*anisole -653.957243			
O	0.3225620	-0.3775380	-1.0494780
O	-2.4036520	-0.8701300	-0.5498210
H	-1.4603080	-0.7957490	-0.7830530
C	-2.5439800	-1.2167300	0.7576770
C	-3.8383820	-1.2437920	1.2847380
C	-1.4526870	-1.5436570	1.5688970
C	-4.0350040	-1.5930810	2.6178070
H	-4.6726000	-0.9880130	0.6391370
C	-1.6633000	-1.8883480	2.9035990
H	-0.4474370	-1.5267070	1.1568960
C	-2.9510720	-1.9159060	3.4371090
H	-5.0437370	-1.6110240	3.0192150
H	-0.8098770	-2.1379390	3.5267590
H	-3.1090500	-2.1855040	4.4759070
C	0.8078380	0.5475830	-0.1595360
C	2.1015670	0.5160920	0.3596070
C	-0.0921120	1.5452540	0.2295670
C	2.4881860	1.5000220	1.2750080
H	2.8077390	-0.2517050	0.0675580
C	0.3082450	2.5124000	1.1425670
H	-1.0944140	1.5436770	-0.1879460
C	1.6024760	2.4965110	1.6711970
H	3.4960320	1.4755120	1.6774560
H	-0.3944580	3.2830110	1.4431640
H	1.9123220	3.2535360	2.3835400
C	1.2007980	-1.4051120	-1.4951740
H	0.6242300	-2.0103640	-2.1926620
H	2.0662810	-0.9743740	-2.0069050
H	1.5335920	-2.0246780	-0.6559660

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3a'PQ-mix G = -1361.618572 ifreq = -1531.34			
C	1.0386390	0.2700500	1.6806520
C	2.1674440	-0.2060380	1.0576430
C	2.2359510	-1.6184740	0.5521120
C	0.8915100	-2.2955070	0.4354940
C	-0.2126990	-1.8056520	1.1722290
C	-0.1667470	-0.4830860	1.7257430

H	2.7737360	-1.6338510	-0.4032000
H	1.0264570	1.2887270	2.0616700
H	2.8549090	-2.2036320	1.2497980
N	3.2502760	0.6103700	0.9052930
H	3.0596230	1.5928080	1.0606910
C	4.4471900	0.3431980	0.2011550
C	4.8714720	1.2569970	-0.7701740
C	5.2376790	-0.7730780	0.4929100
C	6.0682310	1.0484060	-1.4501070
H	4.2520130	2.1203270	-0.9960330
C	6.4221900	-0.9865200	-0.2087450
H	4.9407030	-1.4569200	1.2803860
C	6.8440510	-0.0791540	-1.1802170
H	6.3869810	1.7632100	-2.2019860
H	7.0263460	-1.8582860	0.0214610
H	7.7719680	-0.2457550	-1.7170510
C	-1.3464150	0.0536990	2.3076910
C	-1.4275440	-2.5458430	1.2718600
C	-2.5438330	-2.0053880	1.8545330
H	-3.4653970	-2.5767510	1.9052590
C	-2.5081740	-0.6786620	2.3611260
H	-3.4042600	-0.2438820	2.7933290
H	-1.3187240	1.0712980	2.6901280
H	-1.4573040	-3.5449630	0.8436810
H	0.3217920	-1.9287090	-0.8902090
H	0.9303000	-3.3707490	0.2631540
C	-4.5523830	-2.0822010	-1.5675240
C	-3.1794390	-1.9544980	-1.6353410
C	-2.5470580	-0.7512920	-1.2586220
C	-3.3214300	0.3432840	-0.8014400
C	-4.7206390	0.1883880	-0.7537400
C	-5.3295260	-0.9984290	-1.1264170
C	-1.1099160	-0.6402440	-1.3475140
C	-2.6565010	1.5971290	-0.4038280
C	-1.2551340	1.7197980	-0.5207590
C	-0.4317830	0.6030980	-1.0265580
C	-0.6027810	2.8918400	-0.1150910
H	0.4768950	2.9359830	-0.2210410
C	-1.3217720	3.9539880	0.4110450
C	-2.7126290	3.8460800	0.5296020
C	-3.3659990	2.6888250	0.1275900
H	-5.0295100	-3.0122350	-1.8599900
H	-2.5576840	-2.7758150	-1.9768790
H	-5.3480360	1.0080040	-0.4228910
H	-6.4102250	-1.0862490	-1.0791370
H	-0.8140140	4.8592910	0.7280650
H	-3.2889740	4.6694220	0.9399530
H	-4.4423740	2.6389380	0.2439830
O	0.8065760	0.6766390	-1.1039330
O	-0.3701890	-1.6375250	-1.7388210

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3a'PQ-mix 2TS G = -1361.329918 ifreq = -1226.13			
C	-1.1920240	1.2960640	0.5569960
C	-2.3522590	0.9967930	1.3964580
C	-3.6292480	0.6520210	0.8078100
C	-3.7215610	0.4976710	-0.5984130
H	-0.3721150	0.4635900	0.7733740
H	-0.6281780	2.1681530	0.8885280
C	0.9883350	1.8158000	-1.4068900
C	2.1457320	1.1649210	-1.8513450
C	1.1101910	3.0170440	-0.6946110
C	3.4022520	1.6843230	-1.5520900
H	2.0511960	0.2405710	-2.4148240
C	2.3713030	3.5147390	-0.3768080
H	0.2217720	3.5762740	-0.4201140
C	3.5240510	2.8509620	-0.7978910
H	4.2894160	1.1600650	-1.8936380
H	2.4501340	4.4401950	0.1850220
H	4.5044810	3.2442570	-0.5505290
C	-4.9588720	0.1229050	-1.1641520

C	-4.7768150	0.4500770	1.6025960
C	-5.9822980	0.0924750	1.0274710
H	-6.8582500	-0.0588670	1.6498100
C	-6.0710850	-0.0783670	-0.3669170
H	-7.0162470	-0.3637030	-0.8178720
H	-5.0278490	0.0000970	-2.2418180
H	-4.6982170	0.5775600	2.6792760
H	-1.8953430	-0.2545000	1.8692890
H	-2.3802060	1.4887490	2.3679660
C	-1.0036850	-2.6987560	-1.8549850
C	-1.1028760	-2.1451500	-0.5848800
C	0.0467230	-1.7254760	0.0995810
C	1.3245260	-1.8673610	-0.4888780
C	1.3984090	-2.4382950	-1.7657340
C	0.2527410	-2.8432340	-2.4459120
C	-0.1030300	-1.0807180	1.4044660
C	2.5234420	-1.3923310	0.2356810
C	2.3955090	-0.7028510	1.4602260
C	1.0768530	-0.5273240	2.1184230
C	3.5239350	-0.1971760	2.1192450
H	3.3751100	0.3300400	3.0559970
C	4.7912790	-0.3780870	1.5885650
C	4.9330530	-1.0861600	0.3904410
C	3.8193060	-1.5827890	-0.2723780
H	-1.8986020	-3.0136120	-2.3822570
H	-2.0702160	-2.0255510	-0.1060200
H	2.3572970	-2.5616710	-2.2561570
H	0.3438720	-3.2739350	-3.4378390
H	5.6630560	0.0153790	2.1006070
H	5.9203910	-1.2498350	-0.0302960
H	3.9701540	-2.1228560	-1.1997750
O	0.9434700	0.0558390	3.1890210
O	-1.2185640	-1.1745010	2.0548350
C	-2.5696740	0.7460990	-1.4228670
C	-1.3712260	1.1510620	-0.9133480
H	-2.6688990	0.6074550	-2.4972970
N	-0.2688740	1.2798580	-1.7388470
H	-0.3078130	0.7491470	-2.5995050

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3a'PQ-H2O-TS1-mix G = -1438.038607 ifreq = -1312.83

C	0.9406590	0.4571690	1.6468730
C	2.0995490	-0.0582370	1.1059020
C	2.2071180	-1.5202540	0.7844370
C	0.8713540	-2.2097730	0.6575080
C	-0.2532250	-1.6926370	1.3365990
C	-0.2406820	-0.3205930	1.7640700
H	2.8120450	-1.6450780	-0.1203940
H	0.8924880	1.5126890	1.9033250
H	2.7550080	-2.0159330	1.6012970
N	3.1431900	0.7698630	0.8441380
H	2.9209780	1.7575670	0.8813790
C	4.4197460	0.4636090	0.3252330
C	4.9606800	1.3189930	-0.6412360
C	5.1711930	-0.6196490	0.7894410
C	6.2317100	1.0799000	-1.1515340
H	4.3688730	2.1544740	-1.0040490
C	6.4360180	-0.8637380	0.2567860
H	4.7861390	-1.2545110	1.5788710
C	6.9725160	-0.0191300	-0.7132240
H	6.6381950	1.7467450	-1.9050720
H	7.0095400	-1.7107580	0.6195720
H	7.9601760	-0.2102850	-1.1193260
C	-1.4373020	0.2334150	2.3010780
C	-1.4478940	-2.4546860	1.5008430
C	-2.5768670	-1.8926570	2.0320190
H	-3.4837960	-2.4798610	2.1362930
C	-2.5752800	-0.5239370	2.4214540
H	-3.4829900	-0.0783560	2.8168720
H	-1.4388080	1.2805180	2.5934420
H	-1.4484300	-3.4895560	1.1681610

H	0.3666960	-1.8078940	-0.6715070
H	0.9173000	-3.2895310	0.5210950
C	-4.2064810	-2.5544280	-1.5046120
C	-2.8772960	-2.1839240	-1.5462680
C	-2.4791670	-0.8793830	-1.1859410
C	-3.4502450	0.0685740	-0.7822180
C	-4.7999030	-0.3344630	-0.7564330
C	-5.1768580	-1.6199630	-1.1064360
C	-1.0789030	-0.5221000	-1.2298610
C	-3.0312410	1.4341650	-0.4236830
C	-1.6717180	1.8017470	-0.5180960
C	-0.6465040	0.8301180	-0.9452310
C	-1.2528660	3.0916030	-0.1611450
H	-0.1970640	3.3273790	-0.2482520
C	-2.1651560	4.0287680	0.2962000
C	-3.5169380	3.6758940	0.3953770
C	-3.9399450	2.4031050	0.0393040
H	-4.5013080	-3.5608750	-1.7846900
H	-2.1115780	-2.8895340	-1.8520870
H	-5.5716200	0.3677120	-0.4625720
H	-6.2249040	-1.9003020	-1.0775740
H	-1.8374580	5.0249760	0.5752290
H	-4.2428970	4.3994180	0.7530250
H	-4.9927580	2.1645670	0.1358670
O	0.5608380	1.1431210	-0.9963000
O	-0.1690660	-1.3926010	-1.5842110
H	1.8630540	0.1162340	-1.7686730
O	2.5262560	-0.4369730	-2.2283830
H	1.9801440	-1.1222820	-2.6312780

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3a' CQ TS1 G = -1743.839780 ifreq = -1448.14

C	2.3413310	0.4942920	1.5649120
C	3.5504760	0.1079100	1.0346680
C	3.8542050	-1.3400220	0.7781150
C	2.6334090	-2.2290690	0.7546980
C	1.4446800	-1.8090380	1.4005680
C	1.2704160	-0.4239270	1.7354610
H	4.4290470	-1.4294650	-0.1509800
H	2.1577420	1.5469410	1.7678440
H	4.5225920	-1.6991980	1.5756230
N	4.4933160	1.0462830	0.7417270
H	4.1517570	1.9992820	0.7138140
C	5.7579290	0.8419520	0.1410750
C	6.0912920	1.5845480	-0.9965580
C	6.6918520	-0.0411280	0.6916870
C	7.3448080	1.4346990	-1.5839810
H	5.3593270	2.2657380	-1.4208710
C	7.9350980	-0.2022600	0.0842550
H	6.4557070	-0.5797960	1.6030580
C	8.2679850	0.5337760	-1.0527620
H	7.5939920	2.0146920	-2.4667620
H	8.6524420	-0.8932710	0.5153350
H	9.2408390	0.4110510	-1.5169860
C	0.0075630	0.0035020	2.2270540
C	0.3600300	-2.7084820	1.6215160
C	-0.8411360	-2.2658680	2.1097480
H	-1.6633830	-2.9601240	2.2524390
C	-1.0260300	-0.8860430	2.3959690
H	-1.9902960	-0.5359380	2.7524350
H	-0.1346300	1.0598830	2.4421800
H	0.4985580	-3.7550890	1.3613110
H	2.0886000	-2.1630720	-0.5952990
H	2.8447850	-3.2981740	0.7671680
C	-2.6147510	-3.3277880	-1.1890870
C	-1.3024500	-2.9586270	-1.3381550
C	-0.9026420	-1.6083640	-1.1630180
C	-1.8670000	-0.6347080	-0.8379750
C	-3.2283080	-1.0190030	-0.6783690
C	-3.6098720	-2.3711580	-0.8536950
C	0.4769590	-1.2257870	-1.2887900

C	-1.4874310	0.7493770	-0.6646690
C	-0.1533960	1.1548980	-0.8163020
C	0.8878010	0.1700230	-1.1478130
C	0.2075860	2.5008710	-0.6028760
H	1.2505820	2.7758370	-0.7254050
C	-0.7393090	3.4341930	-0.2436500
C	-2.0959470	3.0609100	-0.0856210
C	-2.4698250	1.7092990	-0.2960760
H	-2.9112930	-4.3642810	-1.3257020
H	-0.5420740	-3.6919680	-1.5865640
H	-0.4575760	4.4705040	-0.0784520
O	2.0896130	0.4760850	-1.2287130
O	1.4111210	-2.0993250	-1.5235600
C	-4.2145140	-0.0457530	-0.3224660
C	-5.5624810	-0.4327910	-0.1534970
C	-3.8354010	1.3153410	-0.1264510
C	-6.5234520	0.5512310	0.2090810
C	-4.8068790	2.2718940	0.2386590
C	-6.1579760	1.8587190	0.3995920
H	-7.5587930	0.2471410	0.3361310
H	-6.9008680	2.6008400	0.6787310
C	-3.1032170	4.0095840	0.2838710
C	-4.4041220	3.6309320	0.4381000
C	-4.9813000	-2.7344820	-0.6840540
C	-5.9215960	-1.8031990	-0.3474560
H	-2.8081050	5.0434810	0.4399950
H	-5.1598200	4.3597530	0.7181200
H	-6.9612370	-2.0913970	-0.2189940
H	-5.2632730	-3.7741660	-0.8263320