

Supporting Information for

**Theoretical Study for Evaluating and Discovering Organic Hydride
Compounds as Novel Trifluoromethylation Reagents**

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Contents

Table S1	S2
Coordinate of Reactants	S4
Coordinate of Transition States	S30
Coordinate of Products	S56
Electron spin density of transition states	S79

Table S1. The differences on Gibbs free energies ($\Delta\Delta G^\circ$), enthalpy changes ($\Delta\Delta H^\circ$), entropy changes ($\Delta\Delta S^\circ$), activation free energies ($\Delta\Delta G^\ddagger$), activation enthalpy changes ($\Delta\Delta H^\ddagger$), and activation entropy changes ($\Delta\Delta S^\ddagger$) of $\text{XH}^{+\cdot}$ releasing CF_3^\cdot in acetonitrile between 298.15K and 355 K.

XH	$\Delta\Delta G^\circ$	$\Delta\Delta H^\circ$	$\Delta\Delta S^\circ$	$\Delta\Delta G^\ddagger$	$\Delta\Delta H^\ddagger$	$\Delta\Delta S^\ddagger$
1H	-2.71	-0.17	9.35	-0.28	-0.06	-0.17
2H	-2.55	-0.16	16.66	-0.23	-0.05	-0.15
3H	-2.46	-0.18	7.99	0.00	-0.06	-0.19
4H	-2.59	-0.18	10.8	-0.10	-0.07	-0.22
5H	-2.47	-0.16	9.96	-0.17	-0.05	-0.16
6H	-2.38	-0.17	11.04	-0.09	-0.06	-0.18
7H	-2.48	-0.15	9.45	-0.19	-0.03	-0.08
8H	-2.45	-0.16	16.36	-0.14	-0.05	-0.12
9H	-2.55	-0.16	8.81	-0.24	-0.04	-0.1
10H	-2.40	-0.17	13.54	-0.12	-0.05	-0.12
11H	-2.44	-0.15	14.35	-0.20	-0.04	-0.11
12H	-2.44	-0.17	12.68	-0.19	-0.05	-0.14
13H	-2.48	-0.16	13.36	-0.08	-0.04	-0.13
14H	-2.50	-0.15	12.72	-0.17	-0.04	-0.13
15H	-2.40	-0.18	13.95	-0.24	-0.05	-0.14
16H	-2.45	-0.15	8.86	-0.34	-0.03	-0.07
17H	-2.56	-0.14	10.75	-0.20	-0.04	-0.11
18H	-2.57	-0.13	10.00	-0.37	-0.03	-0.08
19H	-2.50	-0.14	9.45	-0.33	-0.03	-0.08
20H	-2.43	-0.14	9.62	-0.28	-0.03	-0.08
21H	-2.48	-0.12	4.28	-0.38	0.00	-0.01
22H	-2.61	-0.11	2.80	-0.59	0.01	0.01
23H	-2.50	-0.15	9.71	-0.24	-0.04	-0.12
24H	-2.45	-0.14	6.82	-0.20	-0.04	-0.12
25H	-2.35	-0.14	10.58	-0.13	-0.02	-0.08
26H	-2.40	-0.14	11.25	-0.29	-0.02	-0.03
27H	-2.54	-0.12	10.26	-0.30	0.00	0.00
28H	-2.40	-0.13	11.46	-0.22	-0.02	-0.06
29H	-2.42	-0.13	10.79	-0.13	-0.02	-0.06
30H	-2.48	-0.13	10.07	-0.31	-0.01	-0.02
31H	-2.37	-0.15	9.87	-0.15	-0.03	-0.08
32H	-2.44	-0.14	2.17	-0.35	-0.02	-0.04
33H	-2.36	-0.15	11.41	-0.23	-0.01	-0.02
34H	-2.32	-0.19	17.84	-0.23	-0.05	-0.16
35H	-2.50	-0.13	15.88	-0.27	-0.01	-0.04
36H	-2.27	-0.20	17.72	-0.17	-0.05	-0.14
37H	-2.35	-0.15	10.12	-0.25	-0.02	-0.09
38H	-2.43	-0.12	10.70	-0.36	-0.01	-0.01

39H	-2.38	-0.16	10.66	-0.22	-0.04	-0.12
40H	-2.41	-0.14	10.56	-0.28	-0.01	-0.04
41H	-2.38	-0.18	26.36	-0.13	-0.05	-0.16
42H	-2.30	-0.17	23.08	0.05	-0.05	-0.15
43H	-2.38	-0.15	14.77	-0.08	-0.04	-0.13
44H	-2.45	-0.15	14.29	-0.20	-0.03	-0.09
45H	-2.27	-0.16	14.72	0.12	-0.05	-0.13
46H	-2.44	-0.17	7.62	-0.35	-0.06	-0.19
47H	-2.51	-0.12	8.02	-0.46	-0.01	-0.04

Note: $\Delta\Delta G^o = \Delta G^o_{RD}(XH^{*+}) - \Delta G^o_{RD}(XH^{*+})$; $\Delta\Delta H^o = \Delta H^o_{RD}(XH^{*+}) - \Delta H^o_{RD}(XH^{*+})$; $\Delta\Delta S^o = \Delta S^o_{RD}(XH^{*+}) - \Delta S^o_{RD}(XH^{*+})$; $\Delta\Delta G^{\neq} = \Delta G^{\neq}_{RD}(XH^{*+}) - \Delta G^{\neq}_{RD}(XH^{*+})$; $\Delta\Delta H^{\neq} = \Delta H^{\neq}_{RD}(XH^{*+}) - \Delta H^{\neq}_{RD}(XH^{*+})$; $\Delta\Delta S^{\neq} = \Delta S^{\neq}_{RD}(XH^{*+}) - \Delta S^{\neq}_{RD}(XH^{*+})$. The units of $\Delta\Delta G^o$, $\Delta\Delta H^o$, $\Delta\Delta G^{\neq}$ and $\Delta\Delta H^{\neq}$ are kcal/mol, and the units of $\Delta\Delta S^o$ and $\Delta\Delta S^{\neq}$ are cal mol⁻¹ K⁻¹.

Coordinate of Reactants

1H (Charge = 1, Multiplicity = 2):

C	-2.05906300	0.70323700	0.45220600
C	-2.68051200	1.72790400	-0.22486600
N	-3.85350200	1.43272200	-0.85432900
C	-4.53897100	0.25305200	-0.84954400
C	-3.94902600	-0.81027900	-0.20820000
C	-2.61341900	-0.68063000	0.43946300
C	-2.22481100	3.14959700	-0.34016800
C	-5.86689500	0.27363000	-1.54010300
C	-4.57318900	-2.15682100	-0.04043300
O	-4.11132900	-2.96089400	0.73975700
O	-5.62499300	-2.36515400	-0.81330700
C	-7.42076200	-3.67896400	-1.65126400
C	-6.26549200	-3.65849000	-0.68086600
C	-0.83485100	0.85208300	1.29426800
O	-0.44535300	-0.06363400	1.98622200
O	-0.25543600	2.03680300	1.20692100
C	1.39563700	3.64395400	1.79376300
C	0.92903100	2.22701600	2.02000800
C	-1.58631500	-1.69321500	-0.18722300
F	-1.18081800	-2.59184100	0.70369800
F	-0.50066300	-1.06784900	-0.65866200
F	-2.12042500	-2.35917300	-1.22002700
H	-4.29877200	2.20560400	-1.35190200
H	-2.70433300	-1.02353900	1.48289700
H	-1.22892800	3.19038700	-0.78308100
H	-2.91892100	3.71949600	-0.95945600
H	-2.16904600	3.60589400	0.64995700
H	-6.10479300	1.28709600	-1.86459500
H	-5.84993800	-0.38972800	-2.40678000
H	-6.64680700	-0.07918200	-0.86405600
H	-7.93324900	-4.64118400	-1.58009700
H	-8.13657500	-2.88646200	-1.41913000
H	-7.06712900	-3.54895000	-2.67703300
H	-5.52367000	-4.43030800	-0.90093800
H	-6.59099800	-3.77319400	0.35625100
H	2.29244300	3.82694700	2.39027000
H	1.63914500	3.80879400	0.74127200
H	0.62590300	4.35824600	2.09645400
H	0.66153100	2.03877100	3.06278000
H	1.67458100	1.48920800	1.71268900

2H (Charge = 1, Multiplicity = 2):

C	-3.80387200	0.36536500	0.86833900
C	-4.36861300	1.40153800	0.15236100
N	-5.47465100	1.12904600	-0.58534200
C	-6.13960400	-0.05566700	-0.64670500
C	-5.61375600	-1.12229100	0.04845500
C	-4.32939200	-1.03273700	0.80822500
C	-3.84021500	2.79470500	0.15615200

C	-7.40825000	-0.10954800	-1.42570500
C	-6.33466000	-2.35112200	0.04154200
N	-6.93805100	-3.33966000	0.03757800
C	-2.67109700	0.65037600	1.68281700
N	-1.75651600	0.89700700	2.34938000
C	-3.27067400	-1.97160200	0.17744800
F	-2.15068800	-1.96022600	0.89808700
F	-2.97312800	-1.58793000	-1.06351300
F	-3.72657400	-3.22223400	0.13085300
H	-5.87403500	1.90654600	-1.11795300
H	-4.47193400	-1.42165900	1.83018800
H	-2.83059300	2.80150100	-0.26402500
H	-4.47799800	3.45985300	-0.42586000
H	-3.78378400	3.16021200	1.18492500
H	-7.55066100	0.80581900	-2.00019800
H	-7.39495300	-0.96638600	-2.10285600
H	-8.24772200	-0.23090100	-0.73419200

3H (Charge = 1, Multiplicity = 2):

C	-3.77641800	0.60467000	0.65785200
C	-4.40036800	1.61934900	-0.02799000
N	-5.56807900	1.32133900	-0.67104900
C	-6.23495800	0.13319900	-0.69615800
C	-5.65963300	-0.93030300	-0.04143900
C	-4.36065800	-0.76967800	0.67344800
C	-3.96590300	3.04996100	-0.12511200
C	-7.54805900	0.14552800	-1.41612500
C	-6.27679600	-2.29600300	0.11480200
O	-5.95845000	-2.92408200	1.10701300
C	-7.17127500	-2.87115000	-0.94334400
C	-2.55091300	0.74943000	1.52232800
O	-2.40105500	-0.09240600	2.38891900
C	-1.53836000	1.83156200	1.28915400
C	-3.32009800	-1.83187800	0.18331300
F	-2.99471600	-2.68453300	1.15151900
F	-2.18842600	-1.25874200	-0.24797600
F	-3.79555600	-2.55373000	-0.84303400
H	-6.01714800	2.09573600	-1.16226900
H	-4.53054200	-1.04712100	1.72818900
H	-3.01458200	3.12772100	-0.65445600
H	-4.70959400	3.63672300	-0.66591600
H	-3.84851900	3.47820300	0.87192100
H	-7.81318300	1.16584600	-1.69594600
H	-7.49468300	-0.46042700	-2.32319000
H	-8.33670200	-0.25138400	-0.77467100
H	-7.21193300	-3.95107500	-0.79931700
H	-8.18253800	-2.46521900	-0.85106300
H	-6.79577700	-2.63521700	-1.94215500
H	-0.63233900	1.56378600	1.83310000
H	-1.32029000	1.94006700	0.22378800
H	-1.90611200	2.79041300	1.66473800

4H (Charge = 1, Multiplicity = 2):

C	-3.74424200	0.49395000	0.61298700
C	-4.30222200	1.48508300	-0.15865100
N	-5.39647900	1.15139400	-0.90351800
C	-6.11170900	-0.01231400	-0.85656200
C	-5.59309900	-1.03525300	-0.10182600
C	-4.21543800	-0.91644100	0.46536700
C	-3.84287300	2.90486700	-0.28850700
C	-7.38069600	-0.01753400	-1.65215400
C	-6.23603900	-2.37322600	0.14026200
O	-5.50782100	-3.33449300	0.35339600
N	-7.57970700	-2.43290600	0.13494800
C	-2.58166100	0.64903300	1.55462100
O	-1.88126700	-0.33180900	1.77216100
N	-2.39113100	1.85136300	2.12645500
C	-3.19837700	-1.71928900	-0.44181300
F	-2.63429800	-2.71606200	0.23029900
F	-2.21963500	-0.93182200	-0.90598800
F	-3.79777300	-2.23947100	-1.52004400
H	-5.77184000	1.88599100	-1.50624800
H	-4.16438600	-1.42883300	1.43148500
H	-2.76355200	2.97744200	-0.16247000
H	-4.11000900	3.29124500	-1.27477200
H	-4.33312900	3.53072100	0.46456400
H	-7.28624600	0.66458700	-2.49996000
H	-7.60168000	-1.01623100	-2.02594500
H	-8.21697400	0.32558400	-1.03414800
H	-8.15818900	-1.60551200	0.17216200
H	-8.00774800	-3.31639000	0.38204600
H	-3.08958100	2.58058000	2.10130000
H	-1.66280900	1.92329200	2.82594600

5H (Charge = 1, Multiplicity = 2):

C	-2.01146600	0.89383100	0.33958400
C	-2.67405700	1.91429800	-0.27753600
N	-3.84098900	1.66691500	-0.91980700
C	-4.44879800	0.45654100	-0.95272700
C	-3.85057500	-0.61740300	-0.36140200
C	-2.51965500	-0.50816100	0.30272100
C	-4.52328600	-1.94826000	-0.29505300
O	-4.05186400	-2.86014800	0.34539000
O	-5.64907600	-1.98661600	-0.98730200
C	-7.61856000	-3.06290000	-1.78348400
C	-6.37305300	-3.24274500	-0.95172600
C	-0.77091700	1.13703800	1.13311400
O	-0.26932900	0.26233800	1.80190000
O	-0.32529300	2.37646700	1.01594200
C	1.21105400	4.13470000	1.48367900
C	0.87329400	2.69246000	1.76876500
C	-1.47303000	-1.47610800	-0.35493900
F	-1.05196600	-2.39201600	0.51042600
F	-0.40152300	-0.80976200	-0.79989000
F	-1.99178000	-2.11505200	-1.40945400
H	-2.32742400	2.93963700	-0.27864100

H	-4.31002400	2.45170300	-1.37611700
H	-5.40943300	0.40883300	-1.44959200
H	-2.61512800	-0.87545600	1.33855100
H	-8.19033800	-3.99380500	-1.77730400
H	-8.24645100	-2.26740100	-1.37502600
H	-7.36307500	-2.81953800	-2.81754200
H	-5.71798400	-4.02275300	-1.34802000
H	-6.60051200	-3.47426100	0.09199100
H	2.11260400	4.40720800	2.03734500
H	1.39949200	4.28550300	0.41806500
H	0.39814900	4.79346000	1.79833000
H	0.66607000	2.51525900	2.82717000
H	1.66407400	2.00945900	1.44827600

6H (Charge = 1, Multiplicity = 2):

C	-2.29856900	0.66807400	0.80831000
C	-2.93105100	1.68698500	0.15148400
N	-4.06628100	1.39368900	-0.58675800
C	-4.75056300	0.19369100	-0.49236000
C	-4.14839500	-0.85333600	0.14934700
C	-2.78784200	-0.73256200	0.73257800
C	-2.49904100	3.12062400	0.21763300
C	-6.13545700	0.13756800	-1.06300800
C	-4.60734000	2.43500100	-1.47503000
C	-4.79548300	-2.19365800	0.34051900
O	-4.73356600	-2.77809500	1.39680900
O	-5.37112300	-2.65109800	-0.75920000
C	-6.61148900	-4.26418800	-1.99317500
C	-6.00669800	-3.95022500	-0.64709100
C	-1.08697300	0.85406500	1.67402800
O	-0.98234400	0.28591600	2.73606600
O	-0.17117300	1.63770800	1.12876800
C	1.91985300	2.77440000	1.12573900
C	1.03442900	1.83819000	1.91035700
C	-1.79884000	-1.57476600	-0.10467500
F	-2.16444600	-2.85923800	-0.12222900
F	-0.56385300	-1.50052600	0.39866500
F	-1.75158200	-1.14545300	-1.36777900
H	-2.76935900	-1.18697000	1.73545700
H	-1.86917500	3.27710200	1.08977600
H	-1.92493000	3.39406400	-0.67311600
H	-3.36675100	3.77778800	0.29053300
H	-6.66382700	1.07291600	-0.87343600
H	-6.10487000	-0.03783800	-2.14278100
H	-6.69231000	-0.67479100	-0.60230100
H	-3.78532800	3.03816300	-1.85067700
H	-5.11055200	1.95787900	-2.31147100
H	-5.31186200	3.06306400	-0.92179600
H	-7.10084100	-5.23994400	-1.94848600
H	-7.35743300	-3.51402700	-2.26737300
H	-5.84043500	-4.29751000	-2.76655900
H	-5.24370100	-4.67589700	-0.35398500
H	-6.75925100	-3.89615100	0.14365200

H	2.84349700	2.94681600	1.68320600
H	2.17572200	2.34366100	0.15481000
H	1.42461600	3.73580800	0.96848700
H	0.74917000	2.25191500	2.88084300
H	1.49994500	0.86204000	2.07012200

7H (Charge = 1, Multiplicity = 2):

C	-2.00469500	0.62087900	0.48450100
C	-2.66335200	1.64279100	-0.13890000
N	-3.82900100	1.42469300	-0.79492700
C	-4.42499700	0.19120100	-0.80839900
C	-3.83605900	-0.87801000	-0.21838600
C	-2.50610800	-0.78174600	0.45002100
C	-4.51279400	2.52640300	-1.48310100
C	-4.51738100	-2.20487200	-0.15144300
O	-4.04847700	-3.12125400	0.48477800
O	-5.64844500	-2.23807500	-0.83648000
C	-7.62941900	-3.30521400	-1.61580000
C	-6.37774800	-3.49033100	-0.79436000
C	-0.76755100	0.87080400	1.28100200
O	-0.25974900	-0.00316700	1.94630200
O	-0.33026900	2.11435200	1.17150400
C	1.18683000	3.88404700	1.65576900
C	0.86389000	2.43593000	1.92835200
C	-1.46187600	-1.74414800	-0.21299600
F	-1.03728400	-2.66366800	0.64781500
F	-0.39058200	-1.07635200	-0.65850900
F	-1.98158000	-2.38049400	-1.26910400
H	-2.29580100	2.66129900	-0.12794500
H	-5.38767200	0.13640300	-1.30279800
H	-2.60152500	-1.14997100	1.48421400
H	-3.93506100	3.43849700	-1.35655000
H	-4.59631100	2.26731300	-2.54021000
H	-5.50808500	2.63671700	-1.04914500
H	-8.20566700	-4.23333000	-1.60447800
H	-8.25006800	-2.50651700	-1.20249700
H	-7.38158600	-3.06340900	-2.65209800
H	-5.73016800	-4.27411400	-1.19552200
H	-6.59808300	-3.72078800	0.25113200
H	2.08478000	4.16166000	2.21272700
H	1.37477800	4.04577000	0.59165800
H	0.36648600	4.53141600	1.97483400
H	0.65745600	2.24774500	2.98501000
H	1.66223800	1.76404600	1.60312100

8H (Charge = 1, Multiplicity = 2):

C	-4.91507500	0.86781700	0.61524600
C	-5.50837800	1.91610600	-0.03627200
N	-6.63372900	1.70746400	-0.75505800
C	-7.26976100	0.51901200	-0.85189200
C	-6.74623300	-0.58271500	-0.22990300
C	-5.45444300	-0.52863700	0.52967200
C	-7.47062200	-1.81024500	-0.29274400

N	-8.06414000	-2.80314200	-0.33150100
C	-3.75862200	1.12625600	1.40900900
N	-2.82623200	1.33633600	2.06181000
C	-4.40954200	-1.47545800	-0.11096000
F	-3.29040800	-1.48453700	0.60971700
F	-4.10905300	-1.08472400	-1.34846100
F	-4.88418400	-2.71808500	-0.16695400
H	-5.13045300	2.93040700	-0.00020600
H	-7.05048400	2.51131600	-1.23158000
H	-8.19331800	0.50039100	-1.41707200
H	-5.60725500	-0.92756100	1.54714600

9H (Charge = 1, Multiplicity = 2):

C	-4.17090000	0.94988200	0.46191600
C	-4.88474200	1.98465800	-0.06445300
N	-6.08633000	1.75157200	-0.64939700
C	-6.66861800	0.52881100	-0.73299600
C	-6.02900800	-0.56528700	-0.23169000
C	-4.70736000	-0.44204900	0.44896900
C	-6.66558900	-1.92729700	-0.17435200
O	-6.34469900	-2.67323000	0.74151300
N	-7.56000700	-2.21786600	-1.13073800
C	-2.89009800	1.14759000	1.22496500
O	-2.61003700	0.33794800	2.09918100
N	-2.15119500	2.21822700	0.89766700
C	-3.66736000	-1.46216000	-0.10977600
F	-3.28409000	-2.33202000	0.81986600
F	-2.56963900	-0.84503500	-0.56656700
F	-4.16739000	-2.16165300	-1.13752400
H	-4.56747400	3.01989200	-0.03246500
H	-6.59537300	2.55050100	-1.02974500
H	-7.65166100	0.50403900	-1.18757500
H	-4.84553300	-0.75381200	1.50032700
H	-7.67105500	-1.64933800	-1.95889600
H	-7.98544100	-3.13610800	-1.12404100
H	-2.32514500	2.76120300	0.06343200
H	-1.27406100	2.35830400	1.38214900

10H (Charge = 1, Multiplicity = 2):

C	-2.07898600	2.05715000	0.90215500
C	-2.79001200	3.04142200	0.27096500
N	-3.95695200	2.74244100	-0.33740200
C	-4.53538300	1.50467800	-0.31045800
C	-3.90499100	0.47366700	0.30497700
C	-2.54142500	0.64233200	0.89407000
C	-4.59964200	-0.83224100	0.50543800
O	-4.28348300	-1.60123300	1.38354500
O	-5.59171200	-1.01311700	-0.35524600
C	-7.41053200	-2.24732400	-1.26918300
C	-6.36435800	-2.22611300	-0.18214900
C	-1.50266700	-0.18752900	0.10771000
F	-1.83716800	-1.47546900	0.05434000
F	-0.30135700	-0.09180200	0.68124000

F	-1.39550700	0.25886000	-1.14853300
H	-1.13516800	2.29952100	1.37568400
H	-2.47068100	4.07447300	0.22733500
H	-4.46109500	3.49451000	-0.80839600
H	-5.51453000	1.42566100	-0.76493200
H	-2.51751500	0.22216100	1.91197400
H	-8.01477900	-3.15199500	-1.16860000
H	-8.06971500	-1.37932600	-1.19141500
H	-6.94293000	-2.25069400	-2.25671200
H	-5.68213600	-3.07741000	-0.24801400
H	-6.80560000	-2.21063500	0.81796600

11H (Charge = 1, Multiplicity = 2):

C	-4.85260400	1.02340100	0.49162400
C	-5.57226500	2.01007300	-0.12404000
N	-6.78839600	1.73518900	-0.64272300
C	-7.38050300	0.51085800	-0.58599600
C	-6.73739400	-0.52768000	0.01406700
C	-5.37731400	-0.36138500	0.62988100
C	-7.40862700	-1.78686300	0.09204000
N	-7.95320800	-2.80561800	0.16225600
C	-4.36067800	-1.36537700	0.05969200
F	-4.76297300	-2.62125400	0.26104600
F	-3.17555700	-1.20848700	0.65022300
F	-4.19815500	-1.19021900	-1.25342300
H	-3.87310100	1.25102700	0.89520300
H	-5.21928600	3.02767600	-0.22943200
H	-7.30139900	2.49050100	-1.09991200
H	-8.36617200	0.42817700	-1.02606900
H	-5.43337100	-0.61001600	1.70556200

12H (Charge = 1, Multiplicity = 2):

C	-3.70185800	1.37575700	0.80219900
C	-4.32686900	2.37951100	0.11801100
N	-5.46116200	2.11773800	-0.56962300
C	-6.09173700	0.90835500	-0.56913400
C	-5.55291000	-0.14609000	0.09973800
C	-4.21669300	-0.02076100	0.76251500
C	-6.31650000	-1.42359900	0.28829700
O	-5.95811500	-2.17614400	1.17250200
C	-7.49863300	-1.69906100	-0.59530500
C	-3.15768700	-0.87686100	0.03247100
F	-3.53266600	-2.14771000	-0.09084900
F	-2.00115900	-0.84764400	0.69929700
F	-2.93348300	-0.39868300	-1.19765000
H	-2.78219200	1.58407700	1.33601800
H	-3.96856100	3.40009300	0.08949400
H	-5.90047700	2.88464600	-1.07969400
H	-7.04086200	0.87740900	-1.08972800
H	-4.26633800	-0.45014700	1.77509800
H	-7.86127800	-2.70642800	-0.39371600
H	-8.29725900	-0.97997300	-0.38658500
H	-7.22298000	-1.59997000	-1.64878100

13H (Charge = 1, Multiplicity = 2):

C	-4.06279600	1.30128700	0.65066800
C	-4.73053800	2.32761400	0.04727400
N	-5.94012800	2.10617100	-0.51555700
C	-6.58494800	0.90246700	-0.48802800
C	-5.99525500	-0.17524300	0.08851800
C	-4.62837900	-0.07457300	0.68523500
C	-6.74674500	-1.46019800	0.31537300
O	-6.59068200	-2.05029100	1.37528400
N	-7.57478300	-1.84556100	-0.66858800
C	-3.64512500	-1.02446400	-0.02321100
F	-4.10111200	-2.27745300	-0.05030000
F	-2.46572700	-1.02534600	0.60193900
F	-3.43855800	-0.63973700	-1.28780800
H	-3.08760500	1.48080900	1.08781700
H	-4.34884100	3.33845000	-0.01090400
H	-6.41615700	2.89286600	-0.95756400
H	-7.58192100	0.89179300	-0.91157500
H	-4.67051100	-0.44758700	1.72278500
H	-7.56209600	-1.41254000	-1.58148500
H	-8.09888000	-2.70282200	-0.54994000

14H (Charge = 1, Multiplicity = 2):

C	-4.06143900	0.82860400	0.84901400
C	-4.71611000	1.84951800	0.22451100
N	-5.92337500	1.65353900	-0.36111600
C	-6.55808600	0.43208500	-0.30778400
C	-5.98250400	-0.63941100	0.28289600
C	-4.62262100	-0.54731300	0.89454400
C	-6.61582000	2.75383300	-1.03851000
C	-6.74637600	-1.91769600	0.50983800
O	-6.60774300	-2.50250000	1.57506400
N	-7.56482000	-2.30530800	-0.48166400
C	-3.63772600	-1.50160000	0.19927400
F	-4.09831100	-2.75350800	0.17008500
F	-2.46373900	-1.50692900	0.83556300
F	-3.41621000	-1.12158600	-1.06472700
H	-3.09246800	1.01796600	1.29597500
H	-4.31120800	2.85204700	0.16956300
H	-7.55469900	0.41224500	-0.73478700
H	-4.67641100	-0.91096400	1.93382600
H	-5.99239500	3.64405600	-1.00407600
H	-6.80327500	2.45921000	-2.07256600
H	-7.56435900	2.93227800	-0.52802500
H	-7.53699900	-1.87983300	-1.39763800
H	-8.09585700	-3.15821800	-0.36306500

15H (Charge = 1, Multiplicity = 2):

C	-4.93379100	0.74582900	0.72178400
C	-5.55811300	1.82022600	0.17398500
N	-6.69623400	1.65060400	-0.55301500
C	-7.26734200	0.43842000	-0.79195800

C	-6.70906600	-0.68994500	-0.28234000
C	-5.49187400	-0.62723600	0.57384200
C	-4.41898800	-1.60078600	0.07957700
F	-3.36924000	-1.61319700	0.90639800
F	-3.97680800	-1.25988800	-1.13581400
F	-4.90013900	-2.84459800	0.00462200
H	-4.02335200	0.88769800	1.29200800
H	-5.20087600	2.83673600	0.27234800
H	-7.13658300	2.47678700	-0.95673000
H	-8.16164100	0.44308600	-1.40082700
H	-7.16511900	-1.65209300	-0.48379200
H	-5.75080400	-1.01164500	1.57991100

16H (Charge = 1, Multiplicity = 2):

C	-2.80587900	1.50382800	-0.26285400
C	-2.15203400	0.26745400	-0.21001300
C	-2.88797800	-0.90200600	-0.19046900
C	-4.28907400	-0.82195700	-0.21091400
C	-4.96300500	0.41519000	-0.23929800
C	-4.19762500	1.57523700	-0.27812800
N	-5.02469300	-1.99014900	-0.24293400
C	-6.36366200	-2.04245900	-0.34664900
C	-7.10513100	-0.89144500	-0.35976600
C	-6.47162500	0.45140000	-0.21330400
C	-6.98186600	1.07311100	1.09465900
F	-6.53762100	2.32228000	1.25699600
F	-6.58662700	0.36099000	2.15663500
F	-8.31878500	1.11404200	1.10751200
H	-2.22528900	2.41936800	-0.29393500
H	-1.06888600	0.22411000	-0.19516100
H	-2.41174100	-1.87722600	-0.16751700
H	-4.69116500	2.53966500	-0.32410700
H	-4.51074800	-2.87214000	-0.22205400
H	-6.80338000	-3.02890400	-0.41645300
H	-8.18333700	-0.95669000	-0.43813400
H	-6.84850800	1.11630300	-1.00411000

17H (Charge = 1, Multiplicity = 2):

C	-0.75080400	1.43295000	-0.25864700
C	-0.15669600	0.16737200	-0.17533500
C	-0.94672300	-0.96158600	-0.08336400
C	-2.34340300	-0.80873200	-0.06621500
C	-2.95419300	0.46004100	-0.13007700
C	-2.13907000	1.57737100	-0.23006300
N	-3.14545700	-1.92609600	-0.03933100
C	-4.48000800	-1.90568700	-0.17812700
C	-5.17021400	-0.71984300	-0.24520800
C	-4.45373300	0.57407400	0.00659000
C	-4.76139800	1.02850800	1.44842800
F	-6.07748800	1.11983300	1.66340200
F	-4.22234500	2.22143400	1.70275800
F	-4.26651900	0.15597900	2.33430000
C	-6.64677300	-0.84754200	-0.52281100

O	-7.15249100	-1.96325200	-0.55962800
N	-7.32565900	0.28566200	-0.76160800
H	-0.12637000	2.31539900	-0.34549100
H	0.92279000	0.07122300	-0.19277600
H	-0.52051100	-1.95863200	-0.03399500
H	-2.58711500	2.56363400	-0.28844100
H	-2.68617800	-2.83741300	0.01370100
H	-4.98307700	-2.86062900	-0.26167200
H	-4.82089100	1.37603800	-0.64529300
H	-6.93580900	1.21122700	-0.66828100
H	-8.31721300	0.20998100	-0.94718500

18H (Charge = 1, Multiplicity = 2):

C	-0.76794800	1.87127700	-0.22674900
C	-0.15823600	0.61491500	-0.25520500
C	-0.92450500	-0.53636700	-0.20634200
C	-2.32290100	-0.42808300	-0.12169600
C	-2.94472900	0.83687000	-0.08674300
C	-2.15389700	1.97674100	-0.13866900
N	-3.12067500	-1.57550700	-0.11977000
C	-4.45690400	-1.50747500	-0.25376700
C	-5.14859000	-0.32027700	-0.25267500
C	-4.43762800	0.94803900	0.09087700
C	-2.49067100	-2.90025800	-0.05013400
C	-4.72679700	1.28389400	1.56738600
F	-6.04068900	1.34508500	1.80561500
F	-4.19458500	2.45849300	1.90827400
F	-4.21225200	0.34920300	2.37558700
C	-6.62562200	-0.43373800	-0.53202200
O	-7.13495100	-1.54513200	-0.61965800
N	-7.30268200	0.71156800	-0.70771000
H	-0.16328000	2.77023000	-0.27500400
H	0.92055600	0.53374100	-0.32444600
H	-0.44421700	-1.50557400	-0.24555600
H	-2.62848700	2.95198300	-0.11451500
H	-4.98689500	-2.44347700	-0.38345000
H	-4.81400600	1.79858500	-0.48959100
H	-3.27357600	-3.65013300	0.02774600
H	-1.90040300	-3.06466300	-0.95366100
H	-1.84695900	-2.93644200	0.82957200
H	-6.90126000	1.63180300	-0.60887400
H	-8.29288300	0.64803800	-0.90447800

19H (Charge = 1, Multiplicity = 2):

C	-1.44611600	1.54591000	-0.29784600
C	-0.78645000	0.31029300	-0.20766700
C	-1.51778200	-0.85497300	-0.14743500
C	-2.92639600	-0.77488700	-0.16582900
C	-3.60407300	0.46946600	-0.22817200
C	-2.84181900	1.62250700	-0.30582200
N	-3.65477600	-1.92930700	-0.17085000
C	-4.99787500	-1.98898700	-0.29719300
C	-5.73719700	-0.84012800	-0.33651600

C	-5.11002000	0.51571800	-0.16192100
C	-5.55950600	1.10714500	1.18790200
F	-5.09792900	2.34871600	1.34479200
F	-5.11906700	0.37259100	2.21355300
F	-6.89328200	1.15447600	1.26165200
C	-7.14641500	-0.94325200	-0.52799200
N	-8.28978100	-1.01880500	-0.69652800
H	-0.86609500	2.45989400	-0.36305500
H	0.29659900	0.27276400	-0.19734400
H	-1.04471700	-1.83043200	-0.09714100
H	-3.33073200	2.58749500	-0.37687000
H	-3.14530700	-2.81475400	-0.13080300
H	-5.43432000	-2.97668000	-0.37730900
H	-5.50179100	1.20523300	-0.92161100

20H (Charge = 1, Multiplicity = 2):

C	1.34427100	1.44364800	-0.15158100
C	2.03486200	0.22162400	-0.17245400
C	1.33308300	-0.96360100	-0.15808700
C	-0.07572400	-0.91860200	-0.11481100
C	-0.78359900	0.30466300	-0.07058500
C	-0.04871900	1.48084400	-0.10124000
N	-0.77765500	-2.09285700	-0.14607400
C	-2.12194100	-2.17478800	-0.19249900
C	-2.88994000	-1.04818700	-0.14828900
C	-2.29198700	0.31779800	-0.00422800
C	-2.82244300	1.01028200	1.29429600
F	-3.62836400	2.03308000	0.99772300
F	-1.83424900	1.49600300	2.05070400
F	-3.51630200	0.16022200	2.06439600
C	-4.36610200	-1.22865500	-0.24369800
O	-4.91007400	-2.30929100	-0.25938900
O	-4.98145700	-0.05594400	-0.30801300
C	-6.89458200	1.34978400	-0.26128800
C	-6.42746800	-0.08327200	-0.33707900
H	1.90016900	2.37453400	-0.17557800
H	3.11807700	0.21052300	-0.20878300
H	1.83100100	-1.92775500	-0.18969700
H	-0.56817600	2.43367500	-0.08347100
H	-0.24690700	-2.96555300	-0.17385000
H	-2.55112500	-3.16573400	-0.27404600
H	-2.66791900	0.94816400	-0.82262800
H	-7.98668000	1.37525700	-0.27494900
H	-6.54539100	1.81829400	0.66194000
H	-6.52267500	1.92458800	-1.11295200
H	-6.74168700	-0.57680700	-1.26059800
H	-6.77505300	-0.67793300	0.51159100

21H (Charge = 1, Multiplicity = 2):

C	-0.04977700	0.64891600	0.84709300
C	-0.09532900	1.39983500	-0.33451500
C	-1.27143600	1.48801000	-1.05112300
C	-2.41282400	0.80950700	-0.57736100

C	-2.37200300	0.03019000	0.60151300
C	-1.17972100	-0.03373700	1.30437000
N	-3.59681000	0.95113400	-1.24630300
C	-4.80754800	0.50404300	-0.79615000
C	-4.86299800	-0.28801800	0.37363500
C	-3.58214500	-0.77565800	1.00339500
C	-5.97758100	0.88859700	-1.48196100
C	-7.20333100	0.49423100	-0.98565900
C	-7.27114200	-0.27129000	0.18569200
C	-6.10775600	-0.66180400	0.85374500
C	-3.35603300	-2.23025800	0.57318500
F	-4.38205300	-3.01221600	0.92478300
F	-2.25283700	-2.74147700	1.13009200
F	-3.21618000	-2.32108400	-0.75776600
H	0.87288300	0.59191100	1.41414700
H	0.78954900	1.92012200	-0.68291800
H	-1.34220800	2.07619200	-1.96065700
H	-1.12930600	-0.62194500	2.21465500
H	-3.59041700	1.50820400	-2.10310200
H	-3.67924900	-0.80213400	2.09400300
H	-5.89205200	1.49642300	-2.37752100
H	-8.11285200	0.78513800	-1.49879600
H	-8.23677600	-0.56902600	0.57945900
H	-6.17258600	-1.26380600	1.75406200

22H (Charge = 1, Multiplicity = 2):

C	-0.16353300	0.52179400	1.41642100
C	-0.15680400	1.34611400	0.28730100
C	-1.26188300	1.41061900	-0.54011200
C	-2.40584500	0.64178200	-0.23506700
C	-2.41643500	-0.18455100	0.91212400
C	-1.29085000	-0.24039100	1.71900400
N	-3.54136000	0.72932400	-1.02850200
C	-4.78413000	0.32757500	-0.55993200
C	-4.86600000	-0.50643800	0.57917200
C	-3.60661200	-1.05926400	1.18115200
C	-5.96445000	0.78710000	-1.18344600
C	-7.19404700	0.41734800	-0.67241400
C	-7.27506400	-0.41290900	0.44938200
C	-6.11151100	-0.87258200	1.06455100
C	-3.43913500	1.34387300	-2.35780300
C	-3.34406500	-2.45183700	0.60156100
F	-2.24455900	-3.00001700	1.13018500
F	-3.17104600	-2.39997000	-0.72792100
F	-4.36522300	-3.28092100	0.84320100
H	0.70696800	0.47618000	2.06162700
H	0.71466400	1.94886400	0.05806200
H	-1.25305800	2.07801700	-1.39215600
H	-1.29972400	-0.88658100	2.59082100
H	-3.73366000	-1.20912000	2.25829600
H	-5.91900300	1.45720800	-2.03201300
H	-8.09787900	0.78590300	-1.14410400
H	-8.24319600	-0.69878200	0.84570600

H	-6.16813700	-1.52245700	1.93180900
H	-2.46039300	1.11736900	-2.77276700
H	-4.19824200	0.91084800	-3.00318700
H	-3.57859600	2.42590400	-2.28095200

23H (Charge = 1, Multiplicity = 2):

N	0.04629500	-0.84106400	0.36592400
C	0.18216700	0.45906500	-0.08871500
N	-1.00933500	1.12763300	-0.38824300
C	-2.24833400	0.59968200	-0.26254300
C	-2.37150300	-0.72517900	0.19818200
C	-1.16780700	-1.47628700	0.57481800
N	-3.33326700	1.31334200	-0.59206200
C	-4.62495700	0.90278300	-0.16955200
C	-4.82363900	-0.41622600	0.26551000
C	-3.69093000	-1.40099300	0.18782400
C	-5.67475500	1.82670500	-0.13623800
C	-6.92447200	1.41658000	0.30701200
C	-7.13562800	0.10238200	0.72122400
C	-6.08435600	-0.80882700	0.69889000
C	-3.17253200	2.58532400	-1.30960200
O	-1.23271900	-2.60040400	1.03540300
O	1.24189000	1.02410500	-0.22129700
C	1.25217400	-1.59951400	0.70820200
C	-3.82324200	-2.20536300	-1.12181200
F	-4.96589000	-2.89171400	-1.14216600
F	-2.81772000	-3.06830600	-1.27399400
F	-3.81762600	-1.38394100	-2.18098600
H	-0.87583000	2.10639700	-0.62804500
H	-3.73446100	-2.13958300	0.99617400
H	-5.52208000	2.85917300	-0.42351400
H	-7.73545100	2.13574700	0.33797200
H	-8.11352300	-0.20996400	1.07053100
H	-6.23288300	-1.83273200	1.02648000
H	-4.06776400	2.76288700	-1.89917900
H	-3.01253600	3.40167600	-0.60010100
H	-2.32825100	2.49865700	-1.99284100
H	2.11746600	-1.01126400	0.41692500
H	1.26884300	-1.79118300	1.78221800
H	1.23855300	-2.54737900	0.16996300

24H (Charge = 1, Multiplicity = 2):

N	0.04219500	-1.11700600	0.32766200
C	0.18056200	0.22983500	0.03828700
N	-0.99975300	0.99127100	-0.08846800
C	-2.22724300	0.40504200	-0.08972600
C	-2.35980400	-0.93623900	0.31097000
C	-1.16324300	-1.72961700	0.61925400
N	-3.32221400	1.07443400	-0.50731000
C	-4.61478100	0.67193500	-0.08337300
C	-4.81457600	-0.63611700	0.37580100
C	-3.68102600	-1.61381700	0.27059800
C	-5.66743800	1.59149500	-0.10845800

C	-6.92017900	1.19160400	0.33573300
C	-7.12873500	-0.10864200	0.79625100
C	-6.07789900	-1.02125300	0.80805600
C	-3.23075900	2.15495500	-1.50661200
O	-1.24036600	-2.86205500	1.05656500
O	1.26245500	0.75904300	-0.06557900
C	1.27861900	-1.88565900	0.49503300
C	-0.80819400	2.44966000	0.04298200
C	-3.81109300	-2.36705500	-1.06946400
F	-4.95428900	-3.05122500	-1.11767000
F	-2.80645100	-3.22471600	-1.25546600
F	-3.80318800	-1.50590800	-2.09723600
H	-3.72253400	-2.38233300	1.05047100
H	-5.50765100	2.60823200	-0.44698300
H	-7.73725100	1.90456500	0.32825600
H	-8.10988400	-0.41186200	1.14467600
H	-6.23119700	-2.03951900	1.15099600
H	-4.04298800	1.99532300	-2.21533000
H	-3.32987300	3.13874900	-1.04600000
H	-2.27999500	2.06875100	-2.02692000
H	1.97965800	-1.59053100	-0.28270700
H	1.71342800	-1.68950000	1.47744500
H	1.03130300	-2.94039500	0.40337900
H	0.00950200	2.60578200	0.74330900
H	-0.55762300	2.90774400	-0.91346900
H	-1.71715800	2.88382700	0.45334800

25H (Charge = 1, Multiplicity = 2):

C	-2.11118700	0.54063600	0.84479800
C	-2.29383000	1.82475700	1.36977300
C	-3.56425100	2.40349100	1.39985700
C	-4.65179300	1.70367500	0.90889100
C	-4.48687200	0.39420600	0.37166200
C	-3.18498400	-0.16903100	0.34555900
C	-6.02425300	2.30681400	1.02960000
N	-6.98699200	1.67041200	0.14965500
C	-6.82654000	0.47758200	-0.35762800
C	-5.62360000	-0.24955400	-0.19771100
C	-5.60688500	-1.66704100	-0.67318700
O	-4.82004800	-2.49879300	-0.28238300
O	-6.57476400	-1.89289300	-1.55733800
C	-7.46676400	-4.09627600	-1.01913800
C	-6.71593600	-3.25578300	-2.02934600
C	-6.55654300	2.14803900	2.46447700
F	-5.76847700	2.78012600	3.33155100
F	-6.61389400	0.85811100	2.80875400
F	-7.78815200	2.65459700	2.56574400
H	-1.11933300	0.10350600	0.81871500
H	-1.44411500	2.38129100	1.75031300
H	-3.70113100	3.40133300	1.80354400
H	-3.04097200	-1.15338600	-0.07803500
H	-6.00810500	3.37981800	0.81656100
H	-7.86753700	2.15693300	-0.01490700

H	-7.65597900	0.07441100	-0.92779900
H	-7.61209300	-5.10078700	-1.42490500
H	-6.90637800	-4.17902800	-0.08515600
H	-8.44752700	-3.66146200	-0.81129600
H	-7.26740300	-3.15737200	-2.96428500
H	-5.72088700	-3.65506400	-2.23443300

26H (Charge = 1, Multiplicity = 2):

C	-2.41615300	-0.43592800	0.08822800
C	-2.42253900	0.95619600	-0.04881400
C	-3.62681800	1.65299200	-0.15413400
C	-4.82895200	0.96513100	-0.12137400
C	-4.84000300	-0.45052400	0.00932100
C	-3.60568700	-1.13703700	0.11181900
C	-6.11915700	1.73917800	-0.16321600
N	-7.26796100	0.89510700	-0.43330700
C	-7.26359200	-0.41193600	-0.33212400
C	-6.08861900	-1.13800200	-0.05667000
C	-6.19383200	-2.62134900	0.19054600
O	-5.55709100	-3.13670200	1.09911000
N	-7.04279500	-3.28700200	-0.61228900
C	-6.38636200	2.43935900	1.18074800
F	-5.43386200	3.33110500	1.44750600
F	-6.43117500	1.55924500	2.18378800
F	-7.56091100	3.07748200	1.14362200
H	-1.47482300	-0.96845000	0.16532800
H	-1.48600000	1.50249000	-0.07985400
H	-3.62249200	2.73205100	-0.26582100
H	-3.60754600	-2.21541500	0.20553000
H	-6.08125600	2.53157000	-0.91882000
H	-8.14790400	1.36261600	-0.64640500
H	-8.21954500	-0.90510000	-0.47880600
H	-7.44167400	-2.87420400	-1.44425200
H	-7.14486400	-4.28482700	-0.47764600

27H (Charge = 1, Multiplicity = 2):

C	-1.30389400	-0.64215000	0.18809000
C	-1.28934400	0.75070000	0.06541500
C	-2.48450700	1.46744200	-0.01755800
C	-3.69233800	0.79178700	0.01159200
C	-3.72501400	-0.62008500	0.12980700
C	-2.50422400	-1.32838200	0.21696400
C	-4.98433500	1.56370000	0.04412400
N	-6.12589000	0.78364800	-0.43266000
C	-6.12923200	-0.52732700	-0.33671100
C	-4.99246900	-1.27179500	0.03947700
C	-7.25676800	1.51905500	-1.00653900
C	-5.13594100	-2.74824400	0.30321400
O	-4.53568000	-3.25667100	1.24004500
N	-5.97342800	-3.41600200	-0.51178300
C	-5.27522700	1.98510200	1.49871800
F	-6.39923800	2.70117500	1.59354000
F	-4.27442100	2.72585400	1.97220400

F	-5.41224000	0.91146500	2.28353500
H	-0.36973500	-1.18906700	0.25130100
H	-0.34450100	1.28240200	0.03212900
H	-2.47166300	2.54909700	-0.10516300
H	-2.52057900	-2.40790900	0.29919900
H	-4.91874000	2.48080700	-0.54806000
H	-7.05866800	-1.02463700	-0.59986900
H	-6.90336200	2.03350100	-1.90300800
H	-8.04358300	0.81267300	-1.26179000
H	-7.62306900	2.24975400	-0.28612500
H	-6.31268200	-3.02378000	-1.37954400
H	-6.08025200	-4.41208500	-0.36779500

28H (Charge = 1, Multiplicity = 2):

C	-2.42626800	-0.85667200	-0.34111000
C	-2.47166200	0.54039300	-0.43691100
C	-3.69025100	1.22261100	-0.40355900
C	-4.87300500	0.51502300	-0.27633100
C	-4.83928300	-0.90336900	-0.19935000
C	-3.59639400	-1.57796200	-0.22914000
C	-6.17917100	1.25572500	-0.16226900
N	-7.33722100	0.39069100	-0.32708200
C	-7.30305400	-0.91151700	-0.27677100
C	-6.07583500	-1.60703300	-0.15977500
C	-6.12485600	-3.02779900	-0.07146800
N	-6.15270600	-4.18338100	0.00453400
C	-6.31489600	1.92185600	1.21888400
F	-5.35270100	2.82289400	1.40204500
F	-6.23912100	1.01798500	2.19791000
F	-7.49583600	2.53840500	1.31870500
H	-1.47238800	-1.37081700	-0.36618800
H	-1.55087500	1.10395200	-0.54130200
H	-3.71013900	2.30432600	-0.48075000
H	-3.57733700	-2.66183700	-0.17354900
H	-6.24226500	2.06157900	-0.90164600
H	-8.24377000	0.84476500	-0.43997400
H	-8.24757100	-1.43981600	-0.35490400

29H (Charge = 1, Multiplicity = 2):

C	-7.12892600	1.49212600	-0.42972200
C	-6.38260000	2.67257500	-0.43473000
C	-4.99736300	2.61953800	-0.32866500
C	-4.35608700	1.38950100	-0.21648400
C	-5.09592600	0.19265600	-0.20710900
C	-6.49495300	0.26487100	-0.32475800
C	-2.86394000	1.35943400	-0.03668300
N	-2.28929000	0.06558900	-0.33124400
C	-2.95489500	-1.08650300	-0.28484700
C	-4.39147800	-1.08413700	-0.14223000
C	-2.22343100	-2.30917300	-0.38846900
C	-2.88963400	-3.49444000	-0.27450700
C	-4.29307700	-3.50166600	-0.06832600
C	-5.02104200	-2.32110300	-0.01080700

C	-2.49258800	1.69136800	1.41887400
F	-2.89900300	2.91718400	1.74695900
F	-1.16837700	1.62886700	1.59175500
F	-3.05544300	0.82156700	2.26409900
H	-8.20894100	1.53183100	-0.52113300
H	-6.87957100	3.63194000	-0.53081600
H	-4.40956700	3.53185300	-0.33995300
H	-7.08844600	-0.64143500	-0.34845700
H	-2.37180700	2.11167700	-0.66070900
H	-1.27821300	0.02961300	-0.45876300
H	-1.14786300	-2.25953100	-0.52520300
H	-2.34931000	-4.43248900	-0.32887000
H	-4.80913200	-4.44942200	0.03746300
H	-6.09326300	-2.37229100	0.13333900

30H (Charge = 1, Multiplicity = 2):

C	-7.16118700	1.46565500	-0.19973900
C	-6.42755300	2.65329700	-0.24504300
C	-5.03800700	2.61424100	-0.20575700
C	-4.38554200	1.38833800	-0.11951200
C	-5.10957800	0.18897700	-0.06080800
C	-6.51250300	0.24363900	-0.11641100
C	-2.88931600	1.35275900	-0.00527600
N	-2.29289800	0.09063900	-0.42622000
C	-2.95417300	-1.07137000	-0.28163900
C	-4.37459100	-1.07042200	-0.00624200
C	-2.25551400	-2.31094100	-0.41239900
C	-2.91540500	-3.48884700	-0.19573500
C	-4.28851300	-3.48663900	0.14096900
C	-4.99573500	-2.29731600	0.22533000
C	-0.88525900	0.12695800	-0.84024200
C	-2.47737400	1.58458200	1.46106200
F	-2.91246800	2.76974400	1.88735300
F	-1.14855100	1.55427900	1.60417600
F	-2.99187000	0.63846600	2.25428100
H	-8.24464900	1.49523200	-0.24172900
H	-6.93846600	3.60706600	-0.32179200
H	-4.45792400	3.53066400	-0.24855000
H	-7.09780400	-0.66818000	-0.11017600
H	-2.43680900	2.15910200	-0.58774400
H	-1.19776000	-2.31328400	-0.64047800
H	-2.37880900	-4.42805300	-0.26659000
H	-4.79665400	-4.42633800	0.32701300
H	-6.05039200	-2.32780800	0.47001300
H	-0.60204500	1.16453800	-0.99842700
H	-0.25094900	-0.31177500	-0.06639900
H	-0.77301600	-0.42720100	-1.77328800

31H (Charge = 1, Multiplicity = 2):

C	-0.69728400	-1.11852900	0.45568200
C	-0.22607200	0.16728800	0.31854700
C	-1.11423400	1.24659100	0.11816500
C	-2.47087400	1.02387600	0.05904900

C	-2.97633000	-0.28803000	0.22668100
C	-2.08622400	-1.37602300	0.42184800
C	-3.42610100	2.14547300	-0.26739000
N	-4.81519300	1.81081000	0.00530700
C	-5.28921300	0.57747200	0.15511400
C	-4.37629800	-0.52799700	0.24809600
C	-6.69525600	0.36092100	0.25845500
C	-7.17179100	-0.91992900	0.41309000
C	-6.28809000	-2.00835000	0.49414800
C	-4.88475900	-1.82263800	0.42768900
C	-3.97010600	-2.91291200	0.57410500
C	-2.62432400	-2.69217400	0.57839400
C	-3.34064500	2.50221400	-1.75838300
F	-2.12504100	2.95036000	-2.07223400
F	-4.22819800	3.45589100	-2.06427700
F	-3.60540700	1.44004600	-2.52583800
H	-0.01215000	-1.94810900	0.60062700
H	0.83991700	0.36326600	0.36020600
H	-0.72221900	2.25238600	0.00553600
H	-3.17570500	3.05820600	0.28244600
H	-5.47994900	2.58258200	-0.01894400
H	-7.36219400	1.21466000	0.19592300
H	-8.23980900	-1.09323500	0.47597200
H	-6.67744300	-3.01299700	0.62403500
H	-4.37167800	-3.91332000	0.69974900
H	-1.93113000	-3.51779800	0.70820400

32H (Charge = 1, Multiplicity = 2):

C	-6.76396600	0.43913700	0.28559900
C	-7.13297600	-0.87050400	0.00542600
C	-6.20813400	-1.91450300	-0.20692300
C	-4.80616500	-1.66629100	-0.13969800
C	-4.44289100	-0.35071000	0.14726900
C	-5.37560700	0.70835900	0.35507900
C	-3.73579900	-2.56805100	-0.32572400
C	-2.42356500	-2.11213500	-0.22148200
C	-2.09738200	-0.77202300	0.06969600
C	-3.14437100	0.11767700	0.26049000
C	-3.24010800	1.59220000	0.57742900
N	-4.68900000	1.82252600	0.60012300
C	-2.59371800	2.46591800	-0.48998300
F	-2.76564400	3.76155800	-0.21129200
F	-3.11619200	2.23516900	-1.69657600
F	-1.28304500	2.21804600	-0.54701400
H	-7.49923400	1.21944800	0.44066200
H	-8.18974800	-1.10633700	-0.05513400
H	-6.57171800	-2.91350300	-0.42316500
H	-3.93490600	-3.61106100	-0.54981100
H	-1.61346300	-2.81807900	-0.36928600
H	-1.06025300	-0.46327000	0.13934000
H	-2.79321700	1.85887200	1.54180500
H	-5.10112000	2.72755100	0.81317400

33H (Charge = 1, Multiplicity = 2):

C	-4.99245000	2.59409600	1.57639000
C	-5.16838700	3.23605400	0.31838800
C	-5.78738600	2.58627900	-0.70787600
C	-6.25351400	1.25326200	-0.51643000
C	-6.10248600	0.62404700	0.77373300
C	-5.45160900	1.31377100	1.80183600
N	-6.84316500	0.60195700	-1.51960000
C	-7.19709600	-0.80335100	-1.49725300
C	-7.26898200	-1.32424200	-0.10354900
N	-6.64659200	-0.62539300	0.93269500
C	-7.75835900	-2.48883200	0.39872200
C	-7.44209800	-2.51087400	1.79978400
C	-6.76767300	-1.36669500	2.10148700
C	-6.13210900	-1.56540800	-2.29955900
F	-6.44060700	-2.85935500	-2.37470300
F	-4.92963300	-1.45118000	-1.72658000
F	-6.04156300	-1.08166500	-3.54203600
H	-4.48916600	3.12477300	2.37662700
H	-4.79923700	4.24550600	0.17886400
H	-5.92554800	3.04172800	-1.68301000
H	-5.31457400	0.84408000	2.76756600
H	-6.95193500	1.09058500	-2.40766600
H	-8.14619300	-0.94321000	-2.02320100
H	-8.28007800	-3.24868300	-0.16533100
H	-7.70155600	-3.29019300	2.50133800
H	-6.38483600	-0.99705900	3.03936700

34H (Charge = 1, Multiplicity = 2):

C	-7.17744500	-1.22987300	-0.28542700
C	-6.24339800	-2.28989800	-0.48379000
C	-4.88912300	-2.11625500	-0.30985600
C	-4.46537300	-0.83417400	0.07302600
C	-5.40622500	0.23333500	0.27368900
C	-6.78377200	0.03354200	0.09313900
N	-3.24106300	-0.34703800	0.33290400
C	-3.29324700	1.05192600	0.68246400
N	-4.71066300	1.31952100	0.64794000
C	-2.56524700	1.89344600	-0.37754300
F	-1.27022600	1.57761400	-0.39776300
F	-2.68816600	3.18999300	-0.09277600
F	-3.07104600	1.67857800	-1.59131700
H	-8.23124900	-1.43397300	-0.43954300
H	-6.62024600	-3.26205400	-0.78167000
H	-4.17327700	-2.91570500	-0.45746600
H	-7.48653600	0.84339700	0.24664800
H	-2.37632900	-0.87960900	0.31801500
H	-2.84074500	1.26607300	1.65788600
H	-5.10932500	2.22115400	0.89143700

35H (Charge = 1, Multiplicity = 2):

C	-7.16922600	-1.38750100	-0.40414700
C	-6.24927300	-2.44044700	-0.67436500

C	-4.88851600	-2.27828000	-0.53243300
C	-4.44523700	-1.01653200	-0.10423500
C	-5.37108200	0.04423900	0.16683000
C	-6.75497400	-0.14213300	0.01514400
N	-3.20435700	-0.56511400	0.15198200
C	-3.25145900	0.83723500	0.50640500
N	-4.66988500	1.11560400	0.57977400
C	-5.21467200	2.40325800	0.98302300
C	-1.96985700	-1.32771500	0.04595900
C	-2.61024600	1.68110400	-0.61114600
F	-1.32016300	1.37044400	-0.74653800
F	-2.70415000	2.98054200	-0.32543500
F	-3.22159100	1.46050700	-1.77518900
H	-8.22835300	-1.57671200	-0.53998400
H	-6.63786900	-3.39647000	-1.00738400
H	-4.18551600	-3.07455400	-0.74580700
H	-7.45195000	0.66374400	0.21179300
H	-2.72842800	1.05385600	1.44656800
H	-4.51953300	2.87618300	1.67659500
H	-5.36509300	3.04638300	0.11203900
H	-6.16764800	2.23294100	1.48479700
H	-1.23375600	-0.90098900	0.72694200
H	-2.17508600	-2.35868000	0.33636500
H	-1.58761400	-1.30091600	-0.97754900

36H (Charge = 1, Multiplicity = 2):

C	-4.93091100	-0.09937600	0.63553600
C	-4.85339900	0.10012400	-0.80414000
C	-3.62831300	0.03085000	-1.47592700
C	-2.49635300	-0.23149600	-0.72087400
C	-2.57396000	-0.43270100	0.71463000
C	-3.78298100	-0.36705200	1.38897600
N	-1.20555100	-0.36767000	-1.07117600
C	-0.36702600	-0.61251300	0.07473700
N	-1.32624200	-0.68383200	1.14759900
C	-6.21218700	-0.01435000	1.26897700
C	-7.33362000	0.24713900	0.54202400
C	-7.25730500	0.44274000	-0.87509700
C	-6.06159300	0.37191000	-1.52294200
C	0.58728600	0.57398000	0.29286700
F	1.41213200	0.69251500	-0.74766800
F	1.31059600	0.38319000	1.39623900
F	-0.09057500	1.71358100	0.42515000
H	-3.56568400	0.18043800	-2.54789800
H	-3.83673000	-0.51724000	2.46136000
H	-0.84249600	-0.31974100	-2.01824300
H	0.23445100	-1.52352200	-0.02253400
H	-1.06478200	-0.88252200	2.10860200
H	-6.26253300	-0.16405900	2.34304000
H	-8.29888800	0.30996300	1.03339000
H	-8.16630800	0.64975400	-1.43019700
H	-5.99564300	0.51988900	-2.59643000

37H (Charge = 1, Multiplicity = 2):

C	-2.15402400	-0.02720000	-1.52257300
C	-2.07313400	1.28997500	-0.98834500
C	-2.96605200	1.74941300	-0.03367500
C	-3.95984800	0.87578800	0.39468100
C	-4.04710900	-0.45084700	-0.14456800
C	-3.12324200	-0.90510800	-1.11689200
S	-5.17618400	1.16758300	1.59093900
C	-5.90385300	-0.48795100	1.32386300
N	-5.04636700	-1.15950700	0.38192400
C	-7.31774100	-0.35904900	0.74396500
F	-7.83892600	-1.57072000	0.55335700
F	-7.30177700	0.27707100	-0.42690800
F	-8.09768200	0.31789500	1.58477500
H	-1.42934600	-0.33470400	-2.26783900
H	-1.28908800	1.95045900	-1.34144800
H	-2.89385400	2.75375500	0.36721500
H	-3.20673600	-1.91177300	-1.50972600
H	-5.96854100	-1.03780500	2.26874900
H	-5.21341100	-2.13727500	0.14250600

38H (Charge = 1, Multiplicity = 2):

C	-2.15071900	0.43504200	-1.51846200
C	-2.08960800	1.74655900	-0.97738400
C	-2.98372500	2.17757100	-0.00927300
C	-3.95331400	1.28074400	0.42287600
C	-4.01919900	-0.04455400	-0.11508300
C	-3.09599500	-0.46722900	-1.10352300
S	-5.15894400	1.55165600	1.63728100
C	-5.88192900	-0.09584600	1.32985100
N	-4.99141900	-0.79260800	0.42518800
C	-5.21638000	-2.20321400	0.10841600
C	-7.26774400	0.06798600	0.68547900
F	-7.84474600	-1.12070900	0.50651700
F	-7.17366800	0.66586100	-0.50227300
F	-8.05010400	0.80289900	1.47365400
H	-1.43476600	0.14714300	-2.27976400
H	-1.32546300	2.42789000	-1.33453400
H	-2.93131700	3.18067500	0.39801800
H	-3.15627800	-1.46538000	-1.52018800
H	-6.00079700	-0.65269200	2.26545800
H	-5.80805400	-2.64808500	0.90615400
H	-5.74787400	-2.28698500	-0.84327400
H	-4.25172100	-2.70672700	0.04486800

39H (Charge = 1, Multiplicity = 2):

C	-1.85161700	-0.63135000	0.10679500
C	-2.50861300	-1.89122200	-0.02511800
C	-3.87191400	-2.00499200	-0.26388500
C	-4.55748300	-0.81020100	-0.36245000
C	-3.91410600	0.46138700	-0.22988200
C	-2.52777500	0.55921100	0.00713100
O	-5.86419800	-0.63742600	-0.61334900

C	-6.15101900	0.75168900	-0.57767000
N	-4.86423600	1.38336200	-0.38901900
C	-7.05822300	1.00323800	0.63374300
F	-8.21943300	0.37867700	0.47203400
F	-7.27639500	2.30953100	0.76560600
F	-6.47902000	0.55033700	1.74513000
H	-0.78376600	-0.62505600	0.29318500
H	-1.91401200	-2.79341800	0.06461000
H	-4.37304700	-2.95911100	-0.36771300
H	-2.04626800	1.52410500	0.10552900
H	-6.65272700	1.07141100	-1.49604900
H	-4.72897900	2.39338100	-0.39311000

40H (Charge = 1, Multiplicity = 2):

C	-1.81128500	-0.94060500	0.08267600
C	-2.40992200	-2.23058800	0.14405100
C	-3.78040900	-2.42834000	0.01672600
C	-4.53079600	-1.28587800	-0.17314000
C	-3.94713000	0.01321100	-0.24197000
C	-2.55535600	0.19839100	-0.11113700
O	-5.86246400	-1.20194600	-0.34434200
C	-6.20801600	0.16696300	-0.44988700
N	-4.94222900	0.88166600	-0.45346500
C	-4.83658300	2.32411300	-0.62126600
C	-7.03209100	0.52660900	0.79492100
F	-7.38750000	1.81005000	0.75564700
F	-6.31448400	0.31580300	1.89836900
F	-8.12600100	-0.22508500	0.84636900
H	-0.73600600	-0.86339400	0.19562300
H	-1.76822200	-3.09114000	0.29687800
H	-4.23798000	-3.40859000	0.06175900
H	-2.11549600	1.18736900	-0.15514200
H	-6.79176600	0.36025100	-1.35604200
H	-5.65266300	2.65980300	-1.26071500
H	-4.89830000	2.81357300	0.35423400
H	-3.87866300	2.54550400	-1.09123200

41H (Charge = 1, Multiplicity = 2):

C	-5.28987700	-2.34152600	0.53545100
C	-6.66162000	-2.17144900	0.46402900
C	-7.23226200	-0.90550600	0.28991100
C	-6.40952800	0.23642000	0.20029100
C	-4.99968600	0.06851700	0.23343300
C	-4.43603500	-1.22019400	0.39206200
C	-6.93761600	1.54311200	0.15066900
C	-6.08135700	2.64942300	0.18713500
C	-4.70747400	2.49677700	0.25719400
C	-4.14544500	1.19674600	0.25452300
N	-2.81108900	1.00199600	0.32368200
C	-2.21755600	-0.27765800	0.01847200
N	-3.09262700	-1.33994500	0.45356500
C	-1.96743500	-0.38930000	-1.49254600
F	-1.41172900	-1.56664900	-1.79003200

F	-1.15005100	0.58361400	-1.90389700
F	-3.11026000	-0.28662900	-2.18475200
H	-4.85041800	-3.32370700	0.67579200
H	-7.30599800	-3.03958300	0.54876400
H	-8.31003000	-0.78775800	0.25134500
H	-8.01299800	1.68101500	0.11175900
H	-6.50046500	3.64936500	0.16386600
H	-4.04633700	3.35664800	0.28934000
H	-2.19253500	1.80023800	0.41948200
H	-1.24838900	-0.36689400	0.51140900
H	-2.67832500	-2.24707300	0.63904900

42H (Charge = 1, Multiplicity = 2):

C	-5.31171000	-2.29368700	0.27559800
C	-6.67471000	-2.11136900	0.10540400
C	-7.21883500	-0.84053600	-0.08219400
C	-6.37990500	0.29361700	-0.08594500
C	-4.97730900	0.11993000	0.05098600
C	-4.43463800	-1.18045100	0.22495900
C	-6.91034100	1.59931500	-0.15028200
C	-6.06565300	2.70315600	-0.03097000
C	-4.69891800	2.54964200	0.13741700
C	-4.12699200	1.25211300	0.15522900
N	-2.79436700	1.06018000	0.30738500
C	-2.22763100	-0.22982400	-0.02634100
N	-3.09496800	-1.31670500	0.37655800
C	-2.48239100	-2.60175300	0.71112500
C	-1.88151900	2.17331000	0.56423500
C	-1.93496800	-0.30767600	-1.53266200
F	-1.37746300	-1.48358500	-1.83971300
F	-1.09247000	0.66679000	-1.89144100
F	-3.04757200	-0.17769200	-2.26571000
H	-4.91328700	-3.29167000	0.41028100
H	-7.32653500	-2.97804900	0.11675300
H	-8.28905400	-0.70780100	-0.20145100
H	-7.98075300	1.73136000	-0.26833500
H	-6.48089000	3.70411800	-0.07182800
H	-4.06328500	3.42279600	0.21691900
H	-1.26646000	-0.33740700	0.47964900
H	-2.98645400	-3.03385300	1.57721000
H	-2.53850900	-3.29578200	-0.13240600
H	-1.43617200	-2.43057300	0.96179700
H	-0.90423900	1.76750400	0.82147700
H	-1.78238300	2.81155400	-0.31846700
H	-2.25117900	2.76302800	1.40476400

43H (Charge = 1, Multiplicity = 2):

C	-4.93692200	-0.54828700	0.29651900
C	-3.75615300	-1.07814400	-0.32036700
N	-3.69481800	-2.38770800	-0.43540100
C	-4.59514700	-3.37104900	0.12347400
N	-5.67916100	-2.83654300	0.70949900
C	-6.08503500	-1.46082600	0.57616100

C	-2.61601200	-0.27453800	-0.82973400
O	-4.28254300	-4.53252100	0.06120000
C	-5.16960300	0.88784100	0.64321800
O	-6.09407300	1.20357900	1.35691600
O	-4.29492900	1.71064700	0.10131100
C	-3.34136600	3.85976500	-0.26734700
C	-4.46735100	3.12027600	0.41068700
C	-7.10258900	-1.35515000	-0.58072900
F	-7.51950900	-0.10140600	-0.74838500
F	-8.15699300	-2.12936600	-0.33546400
F	-6.54131500	-1.76724700	-1.72410200
H	-2.87655200	-2.80241900	-0.88861700
H	-6.33430600	-3.48865100	1.13047600
H	-6.60150000	-1.12987300	1.48246900
H	-2.97186500	0.42541200	-1.58906800
H	-2.19959600	0.31555000	-0.00896200
H	-1.85090800	-0.92992400	-1.24542300
H	-3.44061800	4.92775200	-0.05990000
H	-2.37295000	3.52148400	0.10929400
H	-3.37525500	3.71161900	-1.34939300
H	-5.44999700	3.42626800	0.04326700
H	-4.44650900	3.23219500	1.49734000

44H (Charge = 1, Multiplicity = 2):

C	-2.77014800	-0.28096300	-0.29866100
C	-3.23737900	1.04405900	-0.10914200
N	-4.54988000	1.19292600	-0.01653400
C	-5.46383700	0.12149900	-0.12365100
N	-5.13155200	-1.09159000	-0.26714100
C	-3.73306700	-1.42233200	-0.29102300
C	-2.37478500	2.25045300	-0.02630000
C	-1.34698900	-0.61332900	-0.62170900
O	-1.08145900	-1.49175100	-1.40783000
O	-0.48132500	0.12968600	0.03972400
C	1.72394200	0.81077800	0.62556000
C	0.92201500	-0.13518300	-0.23250900
C	-3.47058600	-2.33357300	0.92672000
F	-2.18867100	-2.70958400	0.97632900
F	-4.22505600	-3.42616600	0.85989200
F	-3.75653200	-1.69777200	2.06647400
O	-6.69536800	0.57645300	-0.05868000
C	-7.73912000	-0.41356900	-0.13735400
H	-4.94016800	2.12893800	0.11842100
H	-3.51384800	-2.05133800	-1.16782400
H	-1.77986000	2.20137800	0.88987300
H	-1.68166300	2.26550700	-0.87073800
H	-2.98092200	3.15577000	-0.02518200
H	2.78797500	0.64138800	0.44472700
H	1.49087700	1.84984900	0.38017300
H	1.52031400	0.64016300	1.68530700
H	1.11838300	-1.18340500	0.00559500
H	1.09365200	0.02147100	-1.30023500
H	-8.66785400	0.14602000	-0.05617100

H	-7.68113800	-0.93591200	-1.09360900
H	-7.63810800	-1.12321400	0.68554500

45H (Charge = 1, Multiplicity = 2):

C	-4.93649700	-0.51104700	0.31005600
C	-3.76614800	-1.04315900	-0.30381800
N	-3.65480000	-2.36480700	-0.31944400
C	-4.45573500	-3.29349800	0.38384300
N	-5.55336900	-2.77357400	0.92786500
C	-6.05275300	-1.44527200	0.64650700
S	-3.92607700	-4.85205000	0.51447500
C	-2.67091400	-0.24961300	-0.91775600
C	-7.03710200	-1.52366500	-0.53794700
F	-7.53484200	-0.32384800	-0.82675500
F	-8.03880600	-2.35032200	-0.24971500
F	-6.40991200	-1.99156200	-1.62512700
C	-5.20622300	0.93397400	0.58082000
O	-6.21137300	1.26897600	1.16540900
O	-4.26457700	1.73993000	0.13469800
C	-3.25906700	3.87583000	-0.16481800
C	-4.46662100	3.15761200	0.38328200
H	-2.84153300	-2.77269300	-0.78651600
H	-6.13858000	-3.38977000	1.48604000
H	-6.61200100	-1.06806500	1.50655000
H	-3.08013300	0.43760700	-1.66067700
H	-2.19292300	0.35256900	-0.13955500
H	-1.93666100	-0.91190100	-1.37534500
H	-3.37760500	4.94922800	0.00016200
H	-2.34874900	3.54546400	0.34139100
H	-3.15531900	3.69876700	-1.23807100
H	-5.39320700	3.45643200	-0.11305200
H	-4.58310800	3.29743600	1.46076300

46H (Charge = 1, Multiplicity = 2):

C	-5.69590900	-3.52634400	0.74227900
C	-5.86172800	-3.11193200	2.06934500
C	-6.12972000	-1.78483400	2.34971900
C	-6.23106200	-0.89155200	1.27724200
C	-6.08509200	-1.28212500	-0.06265100
C	-5.81246800	-2.61917100	-0.31377600
O	-6.44432000	0.40730200	1.61639000
C	-6.38630200	1.39601700	0.72694700
C	-6.23455500	1.14120400	-0.65942300
C	-6.31355800	-0.27573400	-1.15881800
C	-6.44580800	2.70265400	1.26197500
C	-6.32591500	3.76638700	0.39942600
C	-6.14713700	3.53362500	-0.97636600
C	-6.10979200	2.23044800	-1.49742700
C	-7.71178700	-0.50397100	-1.74725400
F	-7.84037400	-1.74281000	-2.22933900
F	-7.96773000	0.34773800	-2.74426400
F	-8.65507800	-0.32974100	-0.81019200
H	-5.47580800	-4.56625200	0.52713600

H	-5.77230100	-3.82737400	2.87866700
H	-6.25010200	-1.41489800	3.36191000
H	-5.69062800	-2.95390000	-1.33852200
H	-5.61008700	-0.43185800	-1.98359400
H	-6.56624800	2.82419900	2.33279400
H	-6.35856600	4.78145600	0.77692300
H	-6.04058800	4.37505000	-1.65208300
H	-5.98410100	2.07566900	-2.56370100

47H (Charge = 1, Multiplicity = 2):

C	-7.36666100	0.11842400	0.81632500
C	-7.29802800	1.49430900	0.58115900
C	-6.10298700	2.06276400	0.18168200
C	-4.97017400	1.23801800	0.02238600
C	-5.03253100	-0.15478600	0.23707100
C	-6.24511900	-0.69581300	0.63707800
S	-3.51141000	2.05680700	-0.39875900
C	-2.25114900	0.91421600	-0.11016900
C	-2.49614100	-0.45727800	0.11016200
C	-3.86625700	-1.05920800	-0.07155000
C	-0.94695200	1.44906300	-0.06674400
C	0.11433800	0.61105400	0.22020400
C	-0.11867000	-0.74615300	0.45889400
C	-1.41162300	-1.27268500	0.39672700
C	-3.99784100	-1.52561500	-1.52716300
F	-5.16481300	-2.14104700	-1.73688000
F	-3.02391800	-2.37814300	-1.85637600
F	-3.92988900	-0.48594300	-2.37536400
H	-8.30168100	-0.32858200	1.13632200
H	-8.17406700	2.11798000	0.71623400
H	-6.02753600	3.13162900	0.00618400
H	-6.31609600	-1.76559900	0.80611200
H	-3.94380300	-1.96776500	0.53311300
H	-0.78610000	2.50887900	-0.24082800
H	1.12081300	1.01058400	0.26527300
H	0.71221800	-1.40365600	0.69082800
H	-1.57772900	-2.33145900	0.56808000

Coordinate of Transition States

1H (Charge = 1, Multiplicity = 2):

C	-2.04118000	0.64576800	0.41417900
C	-2.58343200	1.64788900	-0.37820600
N	-3.71428000	1.34312100	-1.06102000
C	-4.39316100	0.16987600	-1.04120400
C	-3.86339100	-0.84717900	-0.25863500
C	-2.65126600	-0.62612200	0.42835900
C	-2.05376200	3.03310200	-0.55935100
C	-5.63768000	0.11269100	-1.86520500
C	-4.42579700	-2.22633900	-0.14220300
O	-3.76384500	-3.14019200	0.29919200
O	-5.67872600	-2.33008200	-0.55579700
C	-7.66569700	-3.54216400	-1.04017500
C	-6.26516700	-3.65247400	-0.48885600
C	-0.78091700	0.76254900	1.20776100
O	-0.19549900	-0.22100800	1.60531900
O	-0.39801500	2.01083200	1.42477700
C	1.09313900	3.66096700	2.26791700
C	0.83016900	2.17792500	2.17426000
C	-1.22676500	-1.80168000	-0.82464900
F	-0.70839500	-2.73487200	-0.06845200
F	-0.31534200	-0.96010600	-1.25537000
F	-1.91476700	-2.30841700	-1.82167900
H	-4.10304900	2.08403000	-1.64432400
H	-2.34365400	-1.34172000	1.18671800
H	-0.99548400	2.99769400	-0.82193800
H	-2.60582700	3.55499300	-1.34230000
H	-2.14354500	3.58794900	0.37737700
H	-5.75340700	1.02772900	-2.44690000
H	-5.60272200	-0.74510500	-2.53879900
H	-6.50573700	-0.01314600	-1.21456000
H	-8.14501900	-4.52334700	-1.00650100
H	-8.26190800	-2.84413100	-0.44728700
H	-7.64759000	-3.20024400	-2.07807000
H	-5.64156400	-4.33377000	-1.07319200
H	-6.25413900	-3.97898900	0.55412100
H	2.01417400	3.82855000	2.83121000
H	1.21084100	4.09745500	1.27287800
H	0.27404000	4.16842200	2.78338900
H	0.69609900	1.71761100	3.15648600
H	1.62777700	1.64757900	1.64797600

2H (Charge = 1, Multiplicity = 2):

C	-4.01226500	0.20183200	1.15088400
C	-4.28481600	1.28270400	0.31905500
N	-5.25328100	1.12165800	-0.60913700
C	-6.00084300	0.01164400	-0.79096900
C	-5.73436200	-1.07753000	0.03253700
C	-4.68347600	-1.02718500	0.97281200
C	-3.57778900	2.58838200	0.39075000
C	-7.06775700	0.02258900	-1.82695200

C	-6.51237200	-2.27121600	-0.12021800
N	-7.13887800	-3.23439100	-0.24878200
C	-2.99420200	0.33092400	2.15137000
N	-2.16813300	0.43508100	2.95356600
C	-3.07252000	-2.17764100	-0.17850300
F	-3.51271100	-3.40330300	-0.31720300
F	-1.98217200	-2.11916700	0.54565700
F	-2.93036400	-1.57283800	-1.33139600
H	-5.45088100	1.92066100	-1.21545400
H	-4.57955000	-1.81644400	1.71409600
H	-4.08762100	3.34210500	-0.20899900
H	-3.52064800	2.92370600	1.42872200
H	-2.55602100	2.46087100	0.01862200
H	-7.09194400	0.97232800	-2.36155200
H	-6.89388100	-0.79192400	-2.53564500
H	-8.03579700	-0.14945200	-1.34674700

3H (Charge = 1, Multiplicity = 2):

C	-3.72377700	0.49164400	0.64975600
C	-4.25779000	1.48918900	-0.15425300
N	-5.37508000	1.18290900	-0.85840900
C	-6.06266600	0.01452800	-0.84082500
C	-5.55130900	-1.00817600	-0.05273700
C	-4.33660500	-0.78136400	0.63316600
C	-3.72344500	2.87181700	-0.34977000
C	-7.28743800	-0.03220800	-1.69680600
C	-6.11596700	-2.40020300	0.07882500
O	-5.34410700	-3.27583900	0.42183800
C	-7.57059200	-2.68147500	-0.16203000
C	-2.47245100	0.59623100	1.48385300
O	-1.88710600	-0.44162800	1.72905500
C	-2.00230200	1.91525000	2.02485500
C	-2.90680400	-1.90812400	-0.67262800
F	-2.36819800	-2.86690000	0.03624200
F	-2.00716400	-1.04397900	-1.08596700
F	-3.60076900	-2.38181300	-1.68295400
H	-5.74551500	1.91986700	-1.45766300
H	-4.02249100	-1.51162100	1.37401100
H	-2.66184200	2.83443600	-0.59941900
H	-4.25491700	3.37694800	-1.15786500
H	-3.84370900	3.45762200	0.56492400
H	-7.38099900	0.88384700	-2.28126900
H	-7.23828100	-0.88013300	-2.38253500
H	-8.18065300	-0.13879300	-1.07716500
H	-7.80037200	-3.66217900	0.25480400
H	-8.20288800	-1.91776300	0.29687800
H	-7.77849400	-2.69741200	-1.23594700
H	-1.30410800	1.71910200	2.83891600
H	-1.48068800	2.47692300	1.24390800
H	-2.83921500	2.52069800	2.38050600

4H (Charge = 1, Multiplicity = 2):

C	-3.78849200	0.48240600	0.67679000
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C	-4.30615900	1.46729800	-0.14903200
N	-5.40714900	1.15029600	-0.87527800
C	-6.09577500	-0.01754300	-0.83945400
C	-5.60310200	-1.01733900	-0.01681000
C	-4.37733100	-0.80142200	0.65050500
C	-3.76985900	2.85078600	-0.33623200
C	-7.30829500	-0.09426200	-1.71124700
C	-6.17875500	-2.40162300	0.12363500
O	-5.41022900	-3.34320100	0.27556400
N	-7.51778000	-2.52037300	0.08548500
C	-2.53740800	0.59688400	1.50738400
O	-1.83001500	-0.39475800	1.63675400
N	-2.27242600	1.78805100	2.07232600
C	-2.99251100	-1.83758100	-0.74537600
F	-2.42054500	-2.82194300	-0.10007400
F	-2.11502800	-0.94761900	-1.15272500
F	-3.71225100	-2.27136800	-1.75603900
H	-5.76277600	1.87028400	-1.50437200
H	-4.04399700	-1.53976100	1.37497700
H	-2.68085000	2.85158900	-0.28996900
H	-4.08965800	3.25519300	-1.29851800
H	-4.15262900	3.50674300	0.45267000
H	-7.22234700	0.60998700	-2.54098100
H	-7.43459000	-1.10170200	-2.10690900
H	-8.20072000	0.16753200	-1.13301600
H	-8.12916000	-1.71929700	0.15864000
H	-7.91659400	-3.43700000	0.24269400
H	-2.95987600	2.52670300	2.11674200
H	-1.46978600	1.85136600	2.68544300

5H (Charge = 1, Multiplicity = 2):

C	-2.01455000	0.85099400	0.36195200
C	-2.48710800	1.84115700	-0.47117100
N	-3.58375300	1.60682800	-1.21526200
C	-4.26576800	0.44690600	-1.19377800
C	-3.83331500	-0.57321700	-0.37602200
C	-2.66588100	-0.39923700	0.39575900
C	-4.50560000	-1.90539400	-0.33973300
O	-3.98994700	-2.86256300	0.19139700
O	-5.67743800	-1.90113000	-0.95407200
C	-7.67200500	-2.94338800	-1.73314300
C	-6.37369100	-3.17171000	-0.99942400
C	-0.77906000	1.01789100	1.18337500
O	-0.25954200	0.08196000	1.74740400
O	-0.34210600	2.26666700	1.19582900
C	1.17658000	3.98178100	1.84340700
C	0.87482800	2.50706500	1.94527800
C	-1.20650100	-1.70112400	-0.74878400
F	-1.84623100	-2.13490700	-1.80831200
F	-0.84772500	-2.67858100	0.04218500
F	-0.19320000	-0.93542100	-1.07515100
H	-2.03298300	2.81974100	-0.56593200
H	-3.92149200	2.35302800	-1.82347700

H	-5.14039300	0.38117300	-1.82911300
H	-2.43108600	-1.10600700	1.18801400
H	-8.22415900	-3.88463100	-1.78641400
H	-8.28874700	-2.20846500	-1.21029000
H	-7.48635800	-2.59211600	-2.75103300
H	-5.73065700	-3.89404000	-1.50894400
H	-6.53216100	-3.50959900	0.02771700
H	2.09206200	4.20017500	2.39824000
H	1.32355200	4.27688100	0.80165000
H	0.36318500	4.57406800	2.26937400
H	0.70767100	2.18895200	2.97730400
H	1.66774100	1.89054800	1.51405300

6H (Charge = 1, Multiplicity = 2):

C	-2.40723200	0.69120600	0.96131600
C	-2.95777900	1.69056700	0.17110200
N	-4.07105000	1.39616400	-0.57073800
C	-4.74487300	0.20684800	-0.48478100
C	-4.20808600	-0.80132400	0.30392100
C	-3.00344900	-0.57961100	0.99006600
C	-2.44463400	3.09652700	0.14418000
C	-6.06252200	0.09272000	-1.18531300
C	-4.57588200	2.42215100	-1.51126500
C	-4.77159500	-2.18645100	0.43703000
O	-4.63034400	-2.84067400	1.44390900
O	-5.34315000	-2.62494900	-0.67610000
C	-6.49267100	-4.25670900	-1.97096500
C	-5.85330400	-3.98008600	-0.63235800
C	-1.13712800	0.81393600	1.75236600
O	-0.95092900	0.18136400	2.76574300
O	-0.23860700	1.59850300	1.17358100
C	1.89575400	2.63942600	1.03534300
C	1.04113300	1.69530700	1.84493100
C	-1.58786200	-1.66736200	-0.40264800
F	-1.95381300	-2.92987100	-0.41096500
F	-0.37645700	-1.51075600	0.08426300
F	-1.70351400	-1.12384000	-1.59144400
H	-2.67403700	-1.30239000	1.73372700
H	-1.82923000	3.28155100	1.02015100
H	-1.83332800	3.26933100	-0.74777000
H	-3.27467400	3.80463200	0.14168600
H	-6.62428800	1.02331000	-1.09219200
H	-5.91813400	-0.12531900	-2.24874400
H	-6.64520900	-0.71356800	-0.74915800
H	-3.73521300	2.99817100	-1.88557700
H	-5.05263500	1.92667600	-2.35107100
H	-5.28771000	3.07455000	-1.00132700
H	-6.88512200	-5.27631000	-1.97862800
H	-7.31889100	-3.56576400	-2.15655800
H	-5.76178300	-4.16018400	-2.77745800
H	-5.01473400	-4.65057500	-0.42620700
H	-6.56769000	-4.05332500	0.19142600
H	2.87514400	2.73554100	1.50990400

H	2.03739600	2.26007900	0.02046600
H	1.43698100	3.62998900	0.98284800
H	0.87109800	2.05750700	2.86191200
H	1.47073800	0.69146000	1.90024300

7H (Charge = 1, Multiplicity = 2):

C	-2.04535400	0.59175900	0.56060600
C	-2.59074800	1.59765600	-0.20978800
N	-3.72878400	1.39053200	-0.90130700
C	-4.36883800	0.20128900	-0.86025100
C	-3.86883800	-0.83771500	-0.10938700
C	-2.66174400	-0.67199800	0.59863500
C	-4.29641700	2.46455000	-1.74106900
C	-4.51523900	-2.18361000	-0.08709400
O	-3.96707900	-3.14341100	0.40535100
O	-5.70273400	-2.18932500	-0.67095900
C	-7.68535100	-3.25724500	-1.44474500
C	-6.37592900	-3.47149700	-0.72658600
C	-0.76290500	0.77018400	1.30417300
O	-0.19252200	-0.16230500	1.82300800
O	-0.34455900	2.02605600	1.30326800
C	1.19140700	3.75642100	1.86294600
C	0.91290800	2.27798600	1.97763600
C	-1.24570700	-1.89930000	-0.68658000
F	-0.27180000	-1.09762400	-1.04805000
F	-1.94169800	-2.30972700	-1.72064500
F	-0.81237400	-2.89824900	0.03875900
H	-2.14602900	2.58258300	-0.28691800
H	-5.28223600	0.12511600	-1.43901800
H	-2.36385900	-1.40153500	1.34738400
H	-5.34730700	2.58487000	-1.48109000
H	-3.75016000	3.38448700	-1.54656900
H	-4.19349600	2.17496300	-2.78697100
H	-8.22163500	-4.20724800	-1.50419700
H	-8.30965600	-2.53935600	-0.90739500
H	-7.51563100	-2.89075400	-2.46006400
H	-5.72534900	-4.17551500	-1.25177100
H	-6.51807800	-3.82552300	0.29757600
H	2.13536300	3.98399500	2.36375500
H	1.27351400	4.05579200	0.81527400
H	0.39784100	4.33835500	2.33778500
H	0.81284000	1.95487200	3.01686900
H	1.68527700	1.67215700	1.49679000

8H (Charge = 1, Multiplicity = 2):

C	-4.95289900	0.75447700	0.76321000
C	-5.34030100	1.75785500	-0.10396800
N	-6.38071500	1.54484400	-0.92579800
C	-7.10329300	0.41285300	-0.94072300
C	-6.75202600	-0.61990300	-0.09297600
C	-5.60456700	-0.50264100	0.72820300
C	-7.53126200	-1.82511400	-0.08690100
N	-8.15095800	-2.80027400	-0.07577700

C	-3.85261400	0.97720500	1.65676700
N	-2.96647600	1.14401000	2.37935500
C	-4.07770600	-1.63384400	-0.56374600
F	-2.90977200	-1.14774100	-0.22601200
F	-4.38935100	-1.35011500	-1.80328000
F	-4.17716800	-2.91101900	-0.30637000
H	-4.85873000	2.72666200	-0.15315700
H	-6.65622200	2.29853900	-1.55843000
H	-7.94745200	0.37305300	-1.61871700
H	-5.40290800	-1.24270900	1.49848300

9H (Charge = 1, Multiplicity = 2):

C	-4.15148900	0.92020400	0.32283200
C	-4.73319900	1.74846100	-0.61095700
N	-5.83690600	1.33758300	-1.26427000
C	-6.43770400	0.15214200	-1.04549200
C	-5.89983300	-0.71838300	-0.12393200
C	-4.69358800	-0.36829500	0.52062200
C	-6.44620700	-2.09450900	0.14537200
O	-5.67975400	-2.95895900	0.55048300
N	-7.75180600	-2.28713200	-0.10394400
C	-2.87841400	1.24645100	1.05657900
O	-2.18984500	0.32246300	1.46990600
N	-2.56682700	2.54685900	1.18497800
C	-3.22431700	-1.60458600	-0.66184900
F	-2.35978900	-0.76453100	-1.18248500
F	-3.90831400	-2.21600700	-1.60109100
F	-2.65216900	-2.45026700	0.15506000
H	-4.36071900	2.72940700	-0.88128700
H	-6.24127000	1.95996300	-1.96319000
H	-7.32519200	-0.04739600	-1.63425500
H	-4.33635700	-0.97514000	1.34840000
H	-8.39099200	-1.52132900	-0.26396600
H	-8.14456300	-3.19931400	0.08826100
H	-3.23403500	3.28307800	1.00236300
H	-1.72879500	2.78603300	1.69868400

10H (Charge = 1, Multiplicity = 2):

C	-2.16393300	2.00512900	1.09045200
C	-2.68460900	2.95009500	0.23918500
N	-3.74916000	2.64291500	-0.53241300
C	-4.35805300	1.44499200	-0.51182900
C	-3.87402400	0.46072400	0.32010400
C	-2.72292500	0.70950600	1.10517500
C	-4.46348800	-0.90848300	0.34574500
O	-3.90557300	-1.83568400	0.88835900
O	-5.62150200	-0.97651600	-0.29438800
C	-7.53740800	-2.13157500	-1.10730400
C	-6.24449700	-2.28286400	-0.34411000
C	-1.23092200	-0.46627500	-0.07899100
F	-0.83932900	-1.47369800	0.66195800
F	-0.23651800	0.34360800	-0.35833600
F	-1.83928500	-0.87391800	-1.16913600

H	-1.32385800	2.25835600	1.72440000
H	-2.30476300	3.95982300	0.15174000
H	-4.12097400	3.36230800	-1.15138500
H	-5.21723100	1.31859500	-1.15849600
H	-2.46716000	0.01072400	1.89754500
H	-8.03670200	-3.10163800	-1.16493600
H	-8.20456700	-1.42742900	-0.60424700
H	-7.34892600	-1.77764800	-2.12379400
H	-5.55303900	-2.97350200	-0.83383400
H	-6.40742900	-2.62262300	0.68186000

11H (Charge = 1, Multiplicity = 2):

C	-4.89467900	1.06712600	0.53851700
C	-5.57687200	1.82185100	-0.38493900
N	-6.73321600	1.35697500	-0.90663500
C	-7.28858000	0.18911700	-0.55639400
C	-6.64494600	-0.60555300	0.37398700
C	-5.38245400	-0.20860300	0.88575000
C	-7.23746200	-1.85035200	0.77074100
N	-7.70351300	-2.85649100	1.09776100
C	-4.01585600	-1.46235100	-0.43092600
F	-3.91397700	-0.83177400	-1.57606400
F	-4.61537800	-2.62182400	-0.56541900
F	-2.85662000	-1.57533000	0.16824000
H	-3.97197400	1.44038600	0.96430500
H	-5.25412600	2.79739600	-0.72490600
H	-7.22148500	1.93441100	-1.59156600
H	-8.23538000	-0.06918900	-1.01449800
H	-4.94765900	-0.75784500	1.71701300

12H (Charge = 1, Multiplicity = 2):

C	-3.73995100	1.39652300	0.83569900
C	-4.27929700	2.32885800	-0.01838600
N	-5.37644700	2.01738300	-0.73929100
C	-6.00113400	0.82856200	-0.66389600
C	-5.50151500	-0.15003000	0.16791300
C	-4.31624700	0.11135800	0.90046600
C	-6.10729200	-1.52128600	0.25841700
O	-5.47259000	-2.38530000	0.83124700
C	-7.44369900	-1.76808300	-0.37695300
C	-2.88073400	-1.11236500	-0.31751700
F	-3.52821900	-1.52206400	-1.38424900
F	-2.47948500	-2.11843100	0.42032100
F	-1.88254400	-0.32140200	-0.63748700
H	-2.87275600	1.65251500	1.43109500
H	-3.88991500	3.33068700	-0.14612700
H	-5.76289100	2.72644800	-1.36094800
H	-6.88691800	0.71441700	-1.27701300
H	-4.03377600	-0.57549600	1.69402800
H	-7.76613000	-2.78336900	-0.14920700
H	-8.18044700	-1.04628600	-0.01262400
H	-7.36355800	-1.64541800	-1.46228200

13H (Charge = 1, Multiplicity = 2):

C	-4.26099900	1.50086700	0.47550800
C	-4.90452000	2.21791200	-0.50462400
N	-5.97250200	1.68146100	-1.12983000
C	-6.48025700	0.47224500	-0.82577900
C	-5.88336600	-0.28642800	0.15490800
C	-4.70016800	0.19238600	0.77062700
C	-6.33642500	-1.67531600	0.50843500
O	-5.51005400	-2.47174600	0.93558700
N	-7.63359000	-1.96097700	0.30018400
C	-3.20415400	-1.03802600	-0.33925900
F	-2.65223400	-1.88188000	0.49706700
F	-2.31861100	-0.18738300	-0.81190000
F	-3.83334500	-1.65374900	-1.31250900
H	-3.41086800	1.93402700	0.98678800
H	-4.61679500	3.21458200	-0.81335900
H	-6.42729600	2.22440900	-1.86271600
H	-7.34841100	0.16076200	-1.39391200
H	-4.32247900	-0.32765100	1.64719700
H	-8.32439500	-1.24259500	0.13438800
H	-7.96352000	-2.88319100	0.55315100

14H (Charge = 1, Multiplicity = 2):

C	-4.49785000	0.93420100	1.25286400
C	-5.06426300	1.83817600	0.38838300
N	-5.99741600	1.44815700	-0.51189200
C	-6.42292700	0.16942000	-0.56761800
C	-5.90170000	-0.78320500	0.28041900
C	-4.85984100	-0.42550900	1.16606800
C	-6.53825000	2.44985200	-1.44874100
C	-6.28693000	-2.23510200	0.21963600
O	-5.46605000	-3.07378200	0.57002600
N	-7.51496400	-2.52304300	-0.24584400
C	-3.12500400	-1.29214600	0.04496200
F	-2.24377600	-0.32032100	-0.06832500
F	-3.55862200	-1.67434900	-1.13385000
F	-2.63739900	-2.29467000	0.73438200
H	-3.76423600	1.27498400	1.97246700
H	-4.81264200	2.89205200	0.38503900
H	-7.18071400	-0.04736500	-1.31205000
H	-4.56397700	-1.12784100	1.94046400
H	-6.80226800	3.34364100	-0.88460200
H	-5.77349800	2.68328000	-2.19004100
H	-7.42009800	2.03663900	-1.93288500
H	-8.23363400	-1.82005500	-0.34560200
H	-7.79739800	-3.49418300	-0.26669300

15H (Charge = 1, Multiplicity = 2):

C	-5.14659000	0.42051400	1.14428500
C	-5.34003500	1.57083200	0.41747900
N	-6.20646900	1.56864200	-0.61565800
C	-6.92946200	0.48799900	-0.97306100
C	-6.77585500	-0.69026400	-0.28239500

C	-5.81758400	-0.75984900	0.75319400
C	-4.14890000	-1.76930200	-0.36477900
F	-3.94497200	-1.07385100	-1.46155000
F	-4.53025100	-2.99612600	-0.64075800
F	-3.08994700	-1.75628600	0.41365300
H	-4.45988700	0.42375000	1.98138700
H	-4.84598800	2.51019200	0.62999600
H	-6.33923000	2.43325700	-1.13759200
H	-7.61909600	0.62050400	-1.79656400
H	-7.36176500	-1.55688000	-0.56191200
H	-5.78997400	-1.63219900	1.40134800

16H (Charge = 1, Multiplicity = 2):

C	-2.78807400	1.41774500	-0.18613700
C	-2.23179600	0.13199700	0.00882200
C	-3.02359900	-0.99208400	0.00246200
C	-4.40777500	-0.83897500	-0.20025400
C	-4.98344100	0.43592000	-0.40233200
C	-4.13917000	1.56997000	-0.38521400
N	-5.23606200	-1.93403800	-0.22411500
C	-6.54767700	-1.86447000	-0.44064500
C	-7.16547200	-0.63593900	-0.64331300
C	-6.40090300	0.52725300	-0.56462500
C	-6.89196500	1.16965900	1.60398900
F	-8.19825600	1.22138900	1.73026800
F	-6.33898000	2.34656200	1.79663000
F	-6.36799000	0.25907400	2.39374600
H	-2.13898400	2.28639900	-0.17478300
H	-1.16327400	0.03137800	0.16635200
H	-2.61121600	-1.98508600	0.14984400
H	-4.58187200	2.55055800	-0.52996700
H	-4.81459000	-2.85195100	-0.08672600
H	-7.08234100	-2.80589900	-0.46117000
H	-8.23134700	-0.60077300	-0.82702600
H	-6.83473300	1.48616200	-0.83999100

17H (Charge = 1, Multiplicity = 2):

C	-0.69939300	1.22646700	-0.01484400
C	-0.21529600	-0.09555100	0.11215000
C	-1.07265300	-1.17196200	0.09311400
C	-2.44841800	-0.92843900	-0.05427400
C	-2.95368000	0.38382800	-0.18790300
C	-2.04518500	1.46627400	-0.16007800
N	-3.34604400	-1.96993100	-0.09506100
C	-4.64999100	-1.81379300	-0.26740500
C	-5.20872800	-0.54150600	-0.40065400
C	-4.36701100	0.56921300	-0.29899900
C	-4.72947100	1.16049700	1.91334600
F	-4.16203300	2.33150200	2.08683800
F	-4.14813300	0.23020600	2.63387600
F	-6.02289200	1.20662500	2.13851900
C	-6.69639900	-0.50323100	-0.62936300
O	-7.29690000	-1.54730400	-0.85291300

N	-7.29185200	0.70095700	-0.58568700
H	0.00039700	2.05457000	0.00505300
H	0.85007900	-0.26463100	0.22600600
H	-0.71482200	-2.19188600	0.18842600
H	-2.43238200	2.47606300	-0.25251300
H	-2.97952400	-2.91800700	-0.00815100
H	-5.25989900	-2.70758100	-0.31708100
H	-4.72169400	1.56916600	-0.54172600
H	-6.82730200	1.55337600	-0.31128500
H	-8.29324100	0.73513700	-0.72195000

18H (Charge = 1, Multiplicity = 2):

C	-1.17129500	2.28840900	-0.34378400
C	-0.36058600	1.13841600	-0.25406100
C	-0.90998200	-0.12240300	-0.16498900
C	-2.31095600	-0.25790000	-0.16517100
C	-3.13729500	0.88764200	-0.25785900
C	-2.53993400	2.16487000	-0.34160100
N	-2.91699100	-1.50610300	-0.09505500
C	-4.23718000	-1.63691100	-0.13429700
C	-5.10331200	-0.54500400	-0.22603100
C	-4.55741400	0.73618000	-0.21986600
C	-2.07726000	-2.71189700	-0.00021800
C	-4.82874500	1.29849600	2.01740200
F	-4.43715700	2.54519300	2.14793300
F	-4.05331100	0.47770700	2.68797200
F	-6.09081500	1.14774200	2.34925300
C	-6.56837800	-0.88855000	-0.29234900
O	-6.90927400	-2.06299900	-0.37084900
N	-7.43938200	0.13424000	-0.27141400
H	-0.71071200	3.26755800	-0.41161900
H	0.71894300	1.24405400	-0.25482800
H	-0.26729100	-0.99050300	-0.09732400
H	-3.18659300	3.03480700	-0.40081500
H	-4.63747100	-2.64374000	-0.10856800
H	-5.15870900	1.61955900	-0.42653000
H	-2.72974600	-3.58002400	0.04426300
H	-1.43712300	-2.77062300	-0.88117700
H	-1.47165800	-2.65458000	0.90463800
H	-7.17832000	1.09981200	-0.14361200
H	-8.42548800	-0.08787400	-0.29940600

19H (Charge = 1, Multiplicity = 2):

C	-1.53542400	1.61624800	-0.28341600
C	-0.88241800	0.37720500	-0.08948100
C	-1.59233600	-0.79999800	-0.01578000
C	-2.98962200	-0.74473800	-0.13666200
C	-3.66314700	0.48336600	-0.33822100
C	-2.90311400	1.67354100	-0.40305800
N	-3.74215300	-1.89534300	-0.07856900
C	-5.05716000	-1.93088900	-0.21391500
C	-5.76627300	-0.74256900	-0.42033000
C	-5.08431100	0.48086200	-0.42266800

C	-5.52656300	1.16196100	1.77698100
F	-5.08008700	2.38520400	1.92721100
F	-4.90140500	0.31373100	2.55742000
F	-6.82844300	1.08967300	1.92024400
C	-7.19079700	-0.79156300	-0.56866000
N	-8.34105100	-0.81977900	-0.68474500
H	-0.94744000	2.52566000	-0.33514000
H	0.19795600	0.35400200	0.00342500
H	-1.10399200	-1.75755600	0.13299300
H	-3.42123500	2.61634600	-0.54640100
H	-3.25099200	-2.77877000	0.06506000
H	-5.53626500	-2.90150400	-0.17104600
H	-5.60593000	1.39535600	-0.69742800

20H (Charge = 1, Multiplicity = 2):

C	1.20847300	1.59971000	-0.27141800
C	1.94170500	0.41618300	-0.02484200
C	1.31065400	-0.80104000	0.09344900
C	-0.08783600	-0.84517100	-0.03460200
C	-0.84112900	0.32602400	-0.28273100
C	-0.15942400	1.55873300	-0.39816100
N	-0.76002900	-2.04192700	0.05941900
C	-2.07411000	-2.16189800	-0.06414700
C	-2.86182400	-1.03875700	-0.30079700
C	-2.26137800	0.22266200	-0.37884500
C	-2.97589300	1.06837100	1.63911000
F	-1.90688800	1.43833400	2.30331200
F	-3.62552500	0.11173600	2.26046300
F	-3.75564200	2.08812500	1.36949700
C	-4.33795300	-1.22345300	-0.35634200
O	-4.88034800	-2.30325800	-0.40577400
O	-4.96362700	-0.05187700	-0.30007100
C	-6.87997400	1.31468000	0.01915400
C	-6.40865100	-0.09175000	-0.26088300
H	1.73451500	2.54379200	-0.35865900
H	3.02069300	0.46857900	0.07282400
H	1.86245500	-1.71639500	0.28211700
H	-0.73860700	2.45847500	-0.58145000
H	-0.21022000	-2.88466800	0.22903700
H	-2.49439000	-3.15711800	0.02123700
H	-2.82553000	1.07381000	-0.75258600
H	-7.97202000	1.33154600	0.04713600
H	-6.50088800	1.66122200	0.98349900
H	-6.54185900	2.00040700	-0.76166300
H	-6.76737900	-0.46771700	-1.22283300
H	-6.71181600	-0.79169400	0.52164800

21H (Charge = 1, Multiplicity = 2):

C	-0.06585800	0.42008500	0.98267600
C	-0.04249800	1.17608100	-0.22042100
C	-1.18096300	1.39028300	-0.95377700
C	-2.39975800	0.84270600	-0.49351100
C	-2.44568300	0.09131700	0.71374900

C	-1.24015500	-0.11296900	1.43930500
N	-3.55025400	1.03445100	-1.18768600
C	-4.76512800	0.56724400	-0.80255800
C	-4.85995000	-0.18738200	0.39953200
C	-3.67870000	-0.45887500	1.11964400
C	-5.91699200	0.83651600	-1.57504800
C	-7.12624300	0.35099200	-1.14899100
C	-7.24064700	-0.41182500	0.04450600
C	-6.13239100	-0.67851400	0.80118200
C	-3.32718700	-2.68218600	0.27056700
F	-2.22877800	-3.16325800	0.80666400
F	-3.21256800	-2.55311500	-1.03182000
F	-4.38047300	-3.39764600	0.59384700
H	0.85535400	0.26864900	1.53391500
H	0.89818300	1.59184100	-0.56581900
H	-1.17043700	1.96560200	-1.87379700
H	-1.28099900	-0.69869900	2.35235500
H	-3.50146000	1.57563100	-2.05068700
H	-3.74610500	-0.95742400	2.08515300
H	-5.82157300	1.41871800	-2.48583100
H	-8.01626800	0.55271300	-1.73581100
H	-8.21339000	-0.78191500	0.34806700
H	-6.19426100	-1.26498700	1.71255900

22H (Charge = 1, Multiplicity = 2):

C	-0.12865200	0.44084700	1.38325100
C	-0.10323700	1.21506600	0.19697800
C	-1.21677200	1.37665700	-0.58993300
C	-2.43740500	0.76206600	-0.21215400
C	-2.48109300	0.02121700	1.00498700
C	-1.29979700	-0.14250100	1.77829300
N	-3.57435700	0.88227000	-0.97191600
C	-4.79672400	0.45117200	-0.52008400
C	-4.87554600	-0.29413500	0.69272900
C	-3.69352000	-0.56851200	1.40040500
C	-5.99631900	0.74404000	-1.21702100
C	-7.19314500	0.27499500	-0.73430400
C	-7.27279900	-0.50478400	0.44599500
C	-6.13182400	-0.78039400	1.14603700
C	-3.48382800	1.49651900	-2.30723200
C	-3.27904900	-2.76909200	0.49397500
F	-2.29989200	-3.31264500	1.18086600
F	-2.94435500	-2.59078200	-0.76434600
F	-4.39192200	-3.45839700	0.60428200
H	0.77388900	0.32702200	1.97275600
H	0.81964000	1.70340800	-0.09839700
H	-1.15583700	2.00003900	-1.47100200
H	-1.36408800	-0.73303900	2.68697400
H	-3.75031200	-1.08500600	2.35687600
H	-5.98855100	1.35811400	-2.10682100
H	-8.10364300	0.51743200	-1.27256300
H	-8.23506500	-0.86657300	0.78974600
H	-6.15120100	-1.36524800	2.06051400

H	-2.50299500	1.29283400	-2.72661300
H	-4.21958500	1.03419900	-2.95937300
H	-3.65483000	2.57321300	-2.24290300

23H (Charge = 1, Multiplicity = 2):

N	0.00025700	-0.99324900	0.33373500
C	0.18336100	0.29422600	-0.13262100
N	-0.97156800	1.03370600	-0.40372500
C	-2.23313700	0.58284800	-0.21719900
C	-2.40827800	-0.71025300	0.32112000
C	-1.23958600	-1.56508900	0.59693900
N	-3.28519700	1.34981800	-0.54185300
C	-4.58527100	0.96004800	-0.19760300
C	-4.80226200	-0.33175600	0.33598100
C	-3.68547300	-1.20206800	0.51358600
C	-5.67125600	1.83805200	-0.34673700
C	-6.93892300	1.40952900	-0.00183500
C	-7.17053200	0.11415900	0.49339800
C	-6.11028000	-0.74603200	0.66132900
C	-3.07008900	2.61610800	-1.26237600
O	-1.35717600	-2.69880000	1.01751900
O	1.27577400	0.78212300	-0.30914300
C	1.21984900	-1.76469600	0.58480700
C	-3.93553700	-2.43585500	-1.44321300
F	-2.78955700	-3.03628800	-1.66037200
F	-4.21639000	-1.57120600	-2.38976200
F	-4.91253400	-3.29200900	-1.26270500
H	-0.77919400	1.99151900	-0.68154500
H	-3.81383900	-2.15489400	1.02293800
H	-5.53052700	2.85031800	-0.70082200
H	-7.77004800	2.09789500	-0.11239900
H	-8.17699600	-0.19671300	0.74929300
H	-6.24996100	-1.75005500	1.05011100
H	-3.92951600	2.80541200	-1.89892000
H	-2.92838200	3.43583700	-0.55542100
H	-2.20372300	2.51154900	-1.91347300
H	1.78825200	-1.30270200	1.39322400
H	0.92253300	-2.77182300	0.86311200
H	1.82629400	-1.78623400	-0.32051800

24H (Charge = 1, Multiplicity = 2):

N	0.01067200	-1.16109600	0.26305600
C	0.17354400	0.18521400	-0.01012100
N	-0.98392500	0.98676200	-0.08672600
C	-2.23042000	0.44007100	-0.03384200
C	-2.37915300	-0.88531800	0.43272200
C	-1.19753400	-1.74518200	0.60948300
N	-3.31605700	1.14282500	-0.41531000
C	-4.60261500	0.71103700	-0.06933400
C	-4.78291800	-0.57690100	0.48157500
C	-3.64117900	-1.42072700	0.61631400
C	-5.71427800	1.54629100	-0.26566100
C	-6.96983000	1.09028800	0.08812400

C	-7.16199100	-0.19501400	0.62624200
C	-6.07838600	-1.02170500	0.81553500
C	-3.21163700	2.26590400	-1.37280200
O	-1.28457200	-2.90118900	0.97475900
O	1.26748800	0.68176400	-0.15537200
C	1.23517500	-1.96275600	0.32024400
C	-0.72890400	2.43357100	0.07280700
C	-3.85949300	-2.60555500	-1.37520300
F	-4.69923700	-3.59019700	-1.16200500
F	-2.66472100	-3.04263900	-1.69687300
F	-4.31952000	-1.75871400	-2.26630400
H	-3.73354000	-2.39542500	1.09063800
H	-5.59767500	2.54509500	-0.66615900
H	-7.82286700	1.74589400	-0.05105900
H	-8.15955400	-0.52807400	0.88920900
H	-6.19203900	-2.02223000	1.22119500
H	-3.98746900	2.11915200	-2.12304000
H	-3.34604700	3.22741100	-0.87722100
H	-2.24663200	2.21804000	-1.86831500
H	1.82821900	-1.76830200	-0.57212800
H	1.81426400	-1.70089900	1.20780400
H	0.94393300	-3.00884500	0.36090200
H	0.09279600	2.54032000	0.77821600
H	-0.45406900	2.89937800	-0.87304400
H	-1.61833100	2.90007000	0.48979600

25H (Charge = 1, Multiplicity = 2):

C	-2.25675500	0.88861200	0.93195700
C	-2.54979000	2.19800700	1.37574600
C	-3.83182800	2.67777200	1.28854300
C	-4.84745200	1.85473600	0.74971700
C	-4.56539400	0.52507200	0.31585900
C	-3.23079300	0.06501400	0.41455500
C	-6.17751700	2.34278200	0.67467500
N	-7.10994500	1.60140200	0.06013600
C	-6.89143700	0.33006100	-0.35673200
C	-5.65221000	-0.23930700	-0.23129100
C	-5.49644800	-1.66798300	-0.65767600
O	-4.61976400	-2.40269300	-0.26394900
O	-6.45371500	-2.02742500	-1.51006700
C	-7.10181200	-4.28697800	-0.86360300
C	-6.46332600	-3.41464400	-1.92317300
C	-6.77134600	1.92887600	2.86043600
F	-5.72565700	2.10404900	3.63092000
F	-7.16975200	0.67746400	2.85522400
F	-7.74902000	2.74681100	3.17184000
H	-1.23725800	0.52327700	1.00039700
H	-1.75862800	2.81924700	1.78064100
H	-4.08801900	3.67952100	1.61936800
H	-2.98380000	-0.93411300	0.08497600
H	-6.41933300	3.38583700	0.85622100
H	-8.04282100	1.99448100	-0.05804300
H	-7.74163400	-0.18214700	-0.78595900

H	-7.15433400	-5.31643100	-1.22743800
H	-6.51471600	-4.27581000	0.05753100
H	-8.11658800	-3.94482000	-0.64559600
H	-7.04157200	-3.41379400	-2.84729600
H	-5.43738200	-3.71949700	-2.13796300

26H (Charge = 1, Multiplicity = 2):

C	-2.46384900	-0.18683700	0.13449900
C	-2.53278800	1.20891000	-0.08043500
C	-3.74951700	1.81629500	-0.26361600
C	-4.92660400	1.03333300	-0.23985200
C	-4.86814500	-0.37127300	-0.01073000
C	-3.59734300	-0.96619700	0.17091800
C	-6.19391300	1.65507700	-0.39490600
N	-7.29012100	0.89094800	-0.47054800
C	-7.27798200	-0.45242000	-0.25480100
C	-6.10059300	-1.10624400	-0.01870400
C	-6.13193900	-2.58570700	0.28136200
O	-5.44541500	-3.05725200	1.17753100
N	-6.98066000	-3.30603400	-0.47530900
C	-6.38704700	2.41795200	1.76280700
F	-6.03481900	1.44097300	2.56510400
F	-7.65026700	2.74046400	1.91735000
F	-5.59753100	3.45824900	1.88962400
H	-1.49398100	-0.65292300	0.27466500
H	-1.62096000	1.79543600	-0.10138100
H	-3.83190200	2.88591700	-0.43034400
H	-3.52913700	-2.03170900	0.34642800
H	-6.29465800	2.69154600	-0.70387000
H	-8.18606100	1.34200600	-0.64985100
H	-8.24463400	-0.93947200	-0.27936200
H	-7.42460100	-2.92628000	-1.29935500
H	-7.04149600	-4.30249500	-0.31178900

27H (Charge = 1, Multiplicity = 2):

C	-1.28578500	-0.30778000	0.30848700
C	-1.38918500	1.09470000	0.16656900
C	-2.61649900	1.67814800	-0.02969700
C	-3.76914100	0.86317300	-0.09143300
C	-3.67557200	-0.54623100	0.06601800
C	-2.39708400	-1.11852300	0.26155600
C	-5.04795100	1.45995100	-0.26478900
N	-6.13545500	0.69397000	-0.42829300
C	-6.07216000	-0.66171100	-0.27605000
C	-4.89020600	-1.30177800	-0.02896300
C	-7.45377600	1.31325800	-0.64312000
C	-4.90381300	-2.79279600	0.20923100
O	-4.24022900	-3.28521900	1.11138300
N	-5.71230300	-3.49866700	-0.60300900
C	-5.44057200	2.06263700	1.92155000
F	-5.87107700	0.96056500	2.49477600
F	-6.36897400	2.99351200	1.91697500
F	-4.32705800	2.49048000	2.46667900

H	-0.30791900	-0.75375000	0.45830500
H	-0.49492100	1.70653500	0.21098800
H	-2.72359000	2.75258400	-0.14210700
H	-2.30568700	-2.19025500	0.38049100
H	-5.14396900	2.51176600	-0.52073000
H	-7.02010900	-1.18124200	-0.35624700
H	-7.95065800	0.79600200	-1.46306100
H	-8.03851500	1.21332500	0.27352500
H	-7.31277200	2.36384200	-0.88963300
H	-6.13019800	-3.09644400	-1.43003700
H	-5.75743600	-4.50184000	-0.48092300

28H (Charge = 1, Multiplicity = 2):

C	-2.47901100	-0.70248300	-0.24605400
C	-2.53708700	0.69728300	-0.44020100
C	-3.74952300	1.33871500	-0.50513000
C	-4.93877100	0.58432900	-0.38759100
C	-4.88111800	-0.82268400	-0.18791100
C	-3.62422700	-1.45619600	-0.12114900
C	-6.20718600	1.22225300	-0.41266400
N	-7.32120000	0.47202300	-0.40514600
C	-7.32042700	-0.86792100	-0.20595200
C	-6.12586300	-1.52769700	-0.08340800
C	-6.13833300	-2.94583500	0.13021600
N	-6.12543300	-4.08903300	0.30406400
C	-6.24098200	1.88698100	1.79799700
F	-5.01379000	2.10095000	2.20227100
F	-6.79378500	0.87380000	2.42346700
F	-6.97766600	2.96782600	1.87500800
H	-1.51143900	-1.19031100	-0.19412700
H	-1.61651500	1.26224300	-0.53469200
H	-3.81830700	2.41281100	-0.64579100
H	-3.56956100	-2.52968900	0.02804600
H	-6.32155200	2.26550200	-0.69208200
H	-8.22176200	0.93970000	-0.50752300
H	-8.28526900	-1.35614700	-0.16609800

29H (Charge = 1, Multiplicity = 2):

C	-6.90325700	1.78263500	-0.38521400
C	-6.04258200	2.89551800	-0.44101500
C	-4.68001300	2.70561900	-0.40833000
C	-4.16257100	1.39712100	-0.32429400
C	-5.01938500	0.27132600	-0.25260500
C	-6.40855600	0.49646400	-0.29448300
C	-2.74481900	1.20071600	-0.28244500
N	-2.25004200	-0.03087400	-0.31930900
C	-3.01896700	-1.17449200	-0.20267200
C	-4.42494600	-1.05221400	-0.15532300
C	-2.37590300	-2.42154800	-0.14466600
C	-3.14003400	-3.56068600	-0.02393300
C	-4.54238700	-3.46637700	0.04059400
C	-5.17167100	-2.23988200	-0.02423600
C	-2.46912000	1.62870400	1.94286600

F	-1.21713100	1.98239800	2.11561200
F	-2.72934600	0.47848600	2.52137100
F	-3.29740100	2.56770000	2.33125700
H	-7.97684600	1.93765100	-0.41480500
H	-6.45443800	3.89608700	-0.51117000
H	-3.99114100	3.54410300	-0.44870400
H	-7.09987600	-0.33706000	-0.25955700
H	-2.05512200	2.01333600	-0.49304600
H	-1.23867300	-0.14597500	-0.38491300
H	-1.29219000	-2.46306800	-0.19062700
H	-2.65841500	-4.53097100	0.02574800
H	-5.13632900	-4.36812300	0.14255900
H	-6.25278700	-2.19407700	0.03093100

30H (Charge = 1, Multiplicity = 2):

C	-7.04986600	1.62431700	-0.04121000
C	-6.25609400	2.78224400	-0.14509600
C	-4.88762400	2.66432400	-0.23342400
C	-4.30122600	1.38257900	-0.22124700
C	-5.08609600	0.21571800	-0.10005300
C	-6.48377800	0.36441800	-0.01967700
C	-2.87891100	1.26132000	-0.31194600
N	-2.28443200	0.07608200	-0.42011000
C	-2.99720000	-1.11474200	-0.24906400
C	-4.40248600	-1.06661500	-0.08016700
C	-2.31367100	-2.34428600	-0.25216300
C	-3.01954600	-3.51589600	-0.07694200
C	-4.41063500	-3.48707300	0.10370000
C	-5.08559800	-2.28423000	0.10138400
C	-0.82643500	0.03311200	-0.61072800
C	-2.38544700	1.65187800	1.88920100
F	-2.62845500	0.50686100	2.48623200
F	-3.13666700	2.61687200	2.36112100
F	-1.10852200	1.95861700	1.94045400
H	-8.12870800	1.72223800	0.02211400
H	-6.72368800	3.76043400	-0.15862800
H	-4.24818200	3.53818800	-0.31548000
H	-7.12735500	-0.50377100	0.05406200
H	-2.27835400	2.13330300	-0.55864900
H	-1.24044500	-2.37950300	-0.38379300
H	-2.48943200	-4.46190500	-0.07495200
H	-4.95783300	-4.41228800	0.24776800
H	-6.15872800	-2.27824800	0.24898700
H	-0.46877400	1.05066600	-0.75071900
H	-0.36045600	-0.40834500	0.27243900
H	-0.59744000	-0.56186400	-1.49513400

31H (Charge = 1, Multiplicity = 2):

C	-0.68794400	-0.92207100	0.36987600
C	-0.26237300	0.39962900	0.23843800
C	-1.18239500	1.43449000	0.10954400
C	-2.54946300	1.13922200	0.12412000
C	-2.99246500	-0.20218600	0.25272400

C	-2.04965800	-1.25091300	0.38048900
C	-3.54325700	2.16037800	-0.03869700
N	-4.83315800	1.85558500	0.06023800
C	-5.32403500	0.56181000	0.16142100
C	-4.38411300	-0.48940000	0.26623700
C	-6.69283700	0.31284300	0.17994900
C	-7.12876900	-1.00448700	0.30064000
C	-6.22453200	-2.05861400	0.40655200
C	-4.84359200	-1.82362400	0.39332200
C	-3.86325600	-2.87461200	0.51209300
C	-2.53456400	-2.60264800	0.50863100
C	-3.33308100	2.34336600	-2.31119100
F	-3.47022800	1.13401800	-2.79871600
F	-2.14967900	2.84410400	-2.57074400
F	-4.30032800	3.13867000	-2.70146700
H	0.04454800	-1.71855700	0.46528100
H	0.79890400	0.62217200	0.23410200
H	-0.85523000	2.46381700	-0.00073400
H	-3.28727900	3.21580000	0.00654000
H	-5.51191900	2.61556300	0.01424700
H	-7.39470700	1.13666900	0.09972000
H	-8.19375900	-1.20905500	0.31360100
H	-6.58621400	-3.07763100	0.50350100
H	-4.21963600	-3.89557700	0.60920300
H	-1.80456500	-3.40090000	0.60291500

32H (Charge = 1, Multiplicity = 2):

C	-6.72201600	0.44616000	0.37593700
C	-7.06995400	-0.79703200	-0.21587300
C	-6.14428400	-1.78686700	-0.50638300
C	-4.76706700	-1.58153600	-0.21150900
C	-4.45306000	-0.35694100	0.37182500
C	-5.38864400	0.63988300	0.66435100
C	-3.65925300	-2.44187600	-0.42754500
C	-2.37335800	-2.04316900	-0.07237500
C	-2.09326600	-0.78799500	0.50885800
C	-3.16585200	0.06493700	0.74166100
C	-3.34935000	1.40488900	1.25755700
N	-4.65178000	1.69173500	1.23182700
C	-2.69794700	2.37808600	-0.88141000
F	-2.50934400	3.66836800	-0.74170800
F	-3.76608000	2.11769200	-1.60024000
F	-1.63288800	1.77709900	-1.35522700
H	-7.47952900	1.19386700	0.58272100
H	-8.11444400	-0.97119000	-0.44952600
H	-6.46952300	-2.71800400	-0.95961100
H	-3.81325900	-3.41880200	-0.87646400
H	-1.54824600	-2.72277900	-0.25373900
H	-1.07330500	-0.51260700	0.75612100
H	-2.64097300	2.06261800	1.74716400
H	-5.04738100	2.56495700	1.57225300

33H (Charge = 1, Multiplicity = 2):

C	-4.94239000	2.62899800	1.35119900
C	-5.15695600	3.20163400	0.08990500
C	-5.84820000	2.50286400	-0.88103000
C	-6.33270200	1.22128300	-0.59355000
C	-6.12097800	0.64849600	0.67307500
C	-5.41852700	1.36222800	1.64650400
N	-7.03043600	0.50701100	-1.56070000
C	-7.43428800	-0.75293200	-1.38500600
C	-7.32557300	-1.33108400	-0.10458300
N	-6.63848400	-0.63483200	0.89951700
C	-7.70540400	-2.56719400	0.40965500
C	-7.26129000	-2.60405300	1.73478800
C	-6.60845400	-1.40450600	2.01076300
C	-5.65381100	-1.80434700	-2.27213500
F	-5.53809200	-1.40454900	-3.51590400
F	-5.79828200	-3.10339400	-2.18474600
F	-4.65892700	-1.37108800	-1.53013100
H	-4.39701800	3.17959400	2.10965400
H	-4.77845900	4.19381900	-0.12826000
H	-6.02498400	2.92109800	-1.86693500
H	-5.24685200	0.92709100	2.62423700
H	-7.17809100	0.94786400	-2.46643100
H	-8.06762100	-1.19315600	-2.14931900
H	-8.24176400	-3.33028400	-0.13595200
H	-7.39318900	-3.41064600	2.44112000
H	-6.14072700	-1.06537100	2.92247500

34H (Charge = 1, Multiplicity = 2):

C	-7.12038600	-0.89741300	-0.38891800
C	-6.27524400	-1.98346300	-0.70825100
C	-4.91221600	-1.94359300	-0.47476600
C	-4.41733100	-0.76968800	0.09748800
C	-5.25836300	0.31050900	0.41672000
C	-6.63348700	0.26764200	0.17652800
N	-3.14346500	-0.38968000	0.46571400
C	-3.16280400	0.87985800	0.91735000
N	-4.44686700	1.28420000	0.96085900
C	-2.52014100	1.89588300	-0.95417000
F	-2.44037500	3.19690500	-0.78372700
F	-3.47611300	1.58314300	-1.80592900
F	-1.36615900	1.38739600	-1.32898600
H	-8.18176900	-0.98099700	-0.59551500
H	-6.70966400	-2.87290400	-1.15133700
H	-4.25598700	-2.77080600	-0.71839600
H	-7.27398500	1.10631600	0.42281400
H	-2.29921300	-0.94670700	0.36896700
H	-2.35397600	1.34714500	1.46394200
H	-4.74551700	2.19376800	1.30138800

35H (Charge = 1, Multiplicity = 2):

C	-7.13540700	-1.06864800	-0.73904100
C	-6.28098900	-2.15526300	-1.02748100
C	-4.92936300	-2.12365300	-0.72828200

C	-4.45846200	-0.95807300	-0.12035600
C	-5.30859400	0.12202600	0.16816700
C	-6.67026300	0.08969200	-0.13967600
N	-3.19682900	-0.59714100	0.30772400
C	-3.24938600	0.66904800	0.76935600
N	-4.52929400	1.09474500	0.76167400
C	-4.98744300	2.41093100	1.19029200
C	-1.98464800	-1.39370000	0.15994000
C	-2.54084700	1.72651900	-1.06387900
F	-2.64872200	3.02907200	-0.89811300
F	-3.36861600	1.29817300	-1.99721900
F	-1.29941400	1.38099400	-1.33791900
H	-8.18606600	-1.14506500	-0.99700400
H	-6.69753100	-3.03852500	-1.49923600
H	-4.26727900	-2.95276500	-0.95089400
H	-7.32015600	0.92881000	0.08167700
H	-2.46087700	1.13242300	1.35116700
H	-5.31265800	2.98231000	0.31849200
H	-5.81718600	2.28742300	1.88706500
H	-4.16158400	2.92056800	1.68452700
H	-1.16662900	-0.87282500	0.65546300
H	-2.14164100	-2.36686400	0.62653900
H	-1.76121200	-1.51878100	-0.90157700

36H (Charge = 1, Multiplicity = 2):

C	-4.82279200	-0.03780000	0.59239300
C	-4.69022900	0.09317000	-0.83512600
C	-3.44226500	-0.09611300	-1.46428500
C	-2.37417000	-0.40912300	-0.65696700
C	-2.50398800	-0.53434600	0.75378000
C	-3.70696900	-0.35447300	1.39518600
N	-1.04267100	-0.66010900	-0.94085000
C	-0.36185700	-0.84706700	0.20603900
N	-1.24092000	-0.84999300	1.22556200
C	-6.10755700	0.16244100	1.18202200
C	-7.19151100	0.47433900	0.41091700
C	-7.05975000	0.60654700	-1.00072200
C	-5.84786700	0.42134700	-1.60382300
C	0.45097500	1.19428700	0.43201000
F	-0.63392900	1.94003600	0.42660900
F	1.22180800	1.46240500	-0.59760000
F	1.10252300	1.30409500	1.56699800
H	-3.33675300	0.00391200	-2.53910700
H	-3.80189100	-0.45071100	2.47131700
H	-0.61485300	-0.65464000	-1.86234100
H	0.63575700	-1.26470900	0.26114100
H	-0.98610600	-1.00707000	2.19626900
H	-6.20031100	0.06000100	2.25930900
H	-8.16235300	0.62359900	0.87233200
H	-7.93182700	0.85584400	-1.59656000
H	-5.73914800	0.52019500	-2.67995700

37H (Charge = 1, Multiplicity = 2):

C	-2.40797800	0.26572500	-1.58298800
C	-2.38178800	1.50189700	-0.91015500
C	-3.20686900	1.75525400	0.17367500
C	-4.06542800	0.73192000	0.57823400
C	-4.08823600	-0.49760600	-0.09513500
C	-3.25823900	-0.75126300	-1.18990200
S	-5.20580100	0.72597900	1.90314900
C	-5.72836000	-0.85193800	1.46411600
N	-5.00621700	-1.36274200	0.47603000
C	-7.64567200	-0.29192700	0.26588500
F	-8.36426400	0.57255400	0.93912400
F	-8.31157800	-1.38819900	0.00193500
F	-7.12838100	0.24245200	-0.81714200
H	-1.74779900	0.10805200	-2.42858000
H	-1.70085300	2.27544200	-1.24764200
H	-3.18558100	2.70767300	0.69088000
H	-3.29347500	-1.70800500	-1.69846100
H	-6.34542800	-1.47147400	2.10698100
H	-5.14512700	-2.32005500	0.14973700

38H (Charge = 1, Multiplicity = 2):

C	-2.46141000	0.38481000	-1.77320800
C	-2.34250400	1.70015700	-1.28998300
C	-3.06186800	2.13322100	-0.18725200
C	-3.90874900	1.21193700	0.42890800
C	-4.02827000	-0.09697300	-0.05689000
C	-3.30325100	-0.53253300	-1.16930000
S	-4.93220800	1.44253300	1.82578500
C	-5.54616600	-0.15553600	1.64291500
N	-4.92812700	-0.84751800	0.69388800
C	-5.24374100	-2.24442200	0.38096500
C	-7.47651400	0.32043000	0.44229000
F	-6.96963100	0.76820900	-0.68567400
F	-8.19317400	1.23408700	1.04931000
F	-8.14651500	-0.79269700	0.26340200
H	-1.88407400	0.08308500	-2.64004600
H	-1.67542700	2.39264300	-1.79151600
H	-2.97310200	3.14814200	0.18323200
H	-3.40301300	-1.54671400	-1.53921700
H	-6.14858300	-0.64302000	2.40397000
H	-5.70821700	-2.28422600	-0.60640400
H	-4.31656800	-2.81831400	0.38521500
H	-5.92649200	-2.62422000	1.13834500

39H (Charge = 1, Multiplicity = 2):

C	-1.98213500	-0.38966000	0.30314200
C	-2.54878100	-1.67925500	0.27173500
C	-3.88005000	-1.89480800	-0.06328100
C	-4.59721400	-0.74995600	-0.36368700
C	-4.05035100	0.53073700	-0.33449400
C	-2.71696900	0.74788000	0.00279300
O	-5.91756800	-0.64928500	-0.73861200
C	-6.19005500	0.64495100	-0.86683200

N	-5.09397900	1.37105400	-0.70032200
C	-7.17556800	0.82317900	1.17622800
F	-7.52453300	2.05808200	1.43294500
F	-6.20816300	0.41087400	1.96542000
F	-8.19821500	0.00529800	1.18959200
H	-0.93706500	-0.28437000	0.57224300
H	-1.92573000	-2.53197400	0.51751200
H	-4.33041200	-2.87938900	-0.09087900
H	-2.29060000	1.74326600	0.02578500
H	-7.10372100	0.96963600	-1.35234900
H	-5.05544400	2.38393500	-0.80848500

40H (Charge = 1, Multiplicity = 2):

C	-1.97511700	-0.85745400	0.52419500
C	-2.54231800	-2.14595500	0.47643900
C	-3.85769300	-2.36301400	0.08224500
C	-4.55978900	-1.22033900	-0.25856400
C	-4.01151900	0.05802300	-0.21427100
C	-2.69482300	0.27834700	0.18086500
O	-5.86151500	-1.11719900	-0.68842400
C	-6.11680800	0.18015700	-0.83113600
N	-5.02951100	0.91259800	-0.62878900
C	-4.94291300	2.36605800	-0.74624500
C	-7.12145300	0.47581300	1.19559800
F	-6.95354200	1.73390900	1.53217900
F	-6.42634500	-0.32930600	1.96824600
F	-8.38769100	0.14334100	1.15808300
H	-0.94362100	-0.75144100	0.84105600
H	-1.93278400	-2.99768100	0.75726600
H	-4.30688500	-3.34775300	0.04253400
H	-2.26802100	1.27387300	0.21561100
H	-7.01140500	0.51012600	-1.34850800
H	-4.68063600	2.77979300	0.22820900
H	-4.17293100	2.60652800	-1.47964000
H	-5.91122700	2.74205200	-1.07226900

41H (Charge = 1, Multiplicity = 2):

C	-5.29854700	-2.29107300	0.24308700
C	-6.69337700	-2.11051900	0.09685400
C	-7.24592300	-0.85888900	-0.02188000
C	-6.42324600	0.30084900	0.00410200
C	-5.02743600	0.12829600	0.15488000
C	-4.48879200	-1.18300300	0.26731300
C	-6.92956500	1.62523900	-0.10678900
C	-6.08053600	2.70395300	-0.06737000
C	-4.68400800	2.53922500	0.08091700
C	-4.17778600	1.26796300	0.18732300
N	-2.80601100	1.02198900	0.34791000
C	-2.28261100	-0.21450600	0.32316800
N	-3.09683200	-1.27806700	0.41791100
C	-1.79081400	-0.33048600	-1.70875600
F	-1.20703400	-1.48176700	-1.92608900
F	-1.01048700	0.68117500	-1.99389800

F	-2.94907800	-0.24334200	-2.31880900
H	-4.86814600	-3.28300000	0.33224400
H	-7.33171500	-2.98751400	0.07696600
H	-8.31811600	-0.73477200	-0.13633600
H	-7.99950100	1.76637500	-0.22264900
H	-6.47904800	3.70929600	-0.15330300
H	-4.01841100	3.39564100	0.10782400
H	-1.24097800	-0.33637300	0.61053600
H	-2.16274200	1.80931300	0.37347700
H	-2.66982700	-2.19813500	0.49248500

42H (Charge = 1, Multiplicity = 2):

C	-5.29492900	-2.29058200	0.23153800
C	-6.68765300	-2.10717800	0.07604700
C	-7.23547500	-0.85538600	-0.04023400
C	-6.40813900	0.29900300	-0.00288500
C	-5.01011000	0.12819800	0.15337700
C	-4.47425000	-1.18619200	0.26523200
C	-6.92552800	1.61797100	-0.10838800
C	-6.08500300	2.70031500	-0.05752600
C	-4.68887100	2.54286700	0.09555000
C	-4.16563200	1.27373200	0.19518700
N	-2.78599100	1.04245600	0.35699000
C	-2.28967500	-0.20844600	0.32774100
N	-3.07943100	-1.29384200	0.42600500
C	-2.46585100	-2.61534400	0.56122000
C	-1.86487900	2.17767200	0.42125800
C	-1.81429300	-0.33205400	-1.71871400
F	-1.25063800	-1.49391900	-1.94922700
F	-1.01893600	0.66415900	-2.02709200
F	-2.97729300	-0.22813100	-2.32007600
H	-4.89146100	-3.29124400	0.31945400
H	-7.32567000	-2.98417700	0.04840500
H	-8.30623600	-0.72464800	-0.16058100
H	-7.99626000	1.74945300	-0.22812600
H	-6.48701500	3.70474300	-0.13748700
H	-4.05113900	3.41699600	0.12888500
H	-1.24643700	-0.33057700	0.61169000
H	-2.88327900	-3.10902900	1.44096100
H	-2.67276200	-3.21248000	-0.32990200
H	-1.39131000	-2.49456500	0.68655300
H	-0.84887900	1.80553800	0.54207300
H	-1.93723100	2.76481000	-0.49699400
H	-2.13101900	2.79891200	1.27882000

43H (Charge = 1, Multiplicity = 2):

C	-4.93091000	-0.56625600	0.25254200
C	-3.79714300	-1.06740900	-0.40020900
N	-3.68708300	-2.39956000	-0.51821700
C	-4.56900800	-3.36592700	-0.01958400
N	-5.64633100	-2.81008600	0.64479900
C	-5.88944600	-1.48258200	0.71965400
C	-2.69550300	-0.25094800	-0.98022000

O	-4.38340900	-4.54878700	-0.14840900
C	-5.29485300	0.86526500	0.42264400
O	-6.41693700	1.19315100	0.74567500
O	-4.29625100	1.70072500	0.19165200
C	-3.34499400	3.86932200	-0.02639600
C	-4.60217800	3.11139800	0.32292200
C	-7.40763700	-1.14665700	-0.83409200
F	-7.00815500	-0.24006700	-1.68839400
F	-8.50063300	-0.79011400	-0.21278000
F	-7.51951500	-2.32647600	-1.39178100
H	-2.87328900	-2.78283500	-0.99923700
H	-6.30340800	-3.46645700	1.06260100
H	-6.65889600	-1.17348000	1.42246600
H	-3.10754200	0.47227400	-1.68712800
H	-2.20486400	0.31332500	-0.18359800
H	-1.96976400	-0.89126500	-1.48109500
H	-3.53471700	4.94145400	0.06402100
H	-2.53018700	3.60266500	0.65122600
H	-3.03692400	3.65675000	-1.05318600
H	-5.42976700	3.34582400	-0.35108500
H	-4.92615900	3.29541400	1.35030300

44H (Charge = 1, Multiplicity = 2):

C	-2.72166600	-0.34686900	-0.13904200
C	-3.22258100	0.89805000	0.21768800
N	-4.56931200	1.03021600	0.18118500
C	-5.40386100	0.02806200	-0.21274700
N	-4.97690100	-1.15169200	-0.57864400
C	-3.64482000	-1.36963500	-0.47904900
C	-2.44182300	2.09751800	0.63232100
C	-1.28886200	-0.74977800	-0.11605300
O	-0.96509800	-1.91786700	-0.11954800
O	-0.44837700	0.27227100	-0.10120300
C	1.72308600	1.23912700	-0.02524800
C	0.96098200	-0.06266600	-0.06610000
C	-3.53936900	-2.56870000	1.33820000
F	-4.76879400	-2.60836400	1.78807100
F	-2.73121200	-1.98894900	2.19092400
F	-3.11002300	-3.75184100	0.98372200
O	-6.66488900	0.36480900	-0.20346600
C	-7.62084400	-0.65816300	-0.56277300
H	-4.98897100	1.92457100	0.43975300
H	-3.26941200	-2.26501400	-0.97154400
H	-1.75252400	1.83217900	1.43561700
H	-1.84512800	2.45285000	-0.21134900
H	-3.11094400	2.89132300	0.96586600
H	2.79479800	1.02824800	-0.00061100
H	1.50825100	1.84188200	-0.91107300
H	1.46147400	1.81349800	0.86698600
H	1.14459200	-0.67917700	0.81745000
H	1.19399200	-0.65160500	-0.95686700
H	-8.59171500	-0.18160700	-0.45310200
H	-7.45449400	-0.97256700	-1.59333200

H -7.52272200 -1.50629000 0.11577400

45H (Charge = 1, Multiplicity = 2):

C	-4.84844100	-0.58267400	0.34871900
C	-3.69367500	-1.07518600	-0.26772500
N	-3.54391600	-2.41171900	-0.32601500
C	-4.38771600	-3.37072000	0.20200300
N	-5.48637400	-2.83271900	0.81307700
C	-5.78202300	-1.51173900	0.83715800
S	-4.07498200	-4.98725100	0.11840200
C	-2.60685900	-0.25577200	-0.86820100
C	-7.30385300	-1.30302100	-0.74958900
F	-6.89030300	-0.44773500	-1.64730500
F	-8.40644800	-0.91712600	-0.16798600
F	-7.39304500	-2.51714900	-1.22939200
C	-5.25981900	0.84394800	0.45409600
O	-6.39581400	1.14503200	0.75176400
O	-4.28594900	1.69810900	0.19537200
C	-3.39622800	3.88345300	-0.10345200
C	-4.63442000	3.10424500	0.26570500
H	-2.70972300	-2.77825200	-0.78489000
H	-6.13240800	-3.48686800	1.25275300
H	-6.57563000	-1.21184800	1.51679700
H	-3.02938600	0.42739400	-1.60795100
H	-2.14195300	0.35243600	-0.08829900
H	-1.85739100	-0.89479300	-1.33442400
H	-3.61814700	4.95228200	-0.05944000
H	-2.58118200	3.66936100	0.59225500
H	-3.07165900	3.63789000	-1.11770400
H	-5.46162300	3.28546600	-0.42486100
H	-4.97372800	3.31941200	1.28199800

46H (Charge = 1, Multiplicity = 2):

C	-5.67866700	-3.52818300	0.65432500
C	-5.97543500	-3.14445400	1.98399800
C	-6.19487700	-1.82646700	2.32752900
C	-6.11513800	-0.86363400	1.31898800
C	-5.81012400	-1.21355100	-0.01810400
C	-5.60078900	-2.58138300	-0.33441300
O	-6.33392600	0.41747100	1.66664700
C	-6.26091100	1.41605700	0.76797500
C	-5.96649900	1.15289200	-0.59129900
C	-5.78694200	-0.18822800	-0.98468800
C	-6.47982100	2.71539500	1.23119200
C	-6.41169500	3.74851700	0.31938900
C	-6.13092700	3.51757900	-1.04849000
C	-5.91500600	2.24142900	-1.50094900
C	-8.11328200	-0.54228300	-1.70182100
F	-8.26433000	-1.78705000	-2.07866600
F	-8.42309300	0.30707700	-2.64840100
F	-8.74989700	-0.28676500	-0.58219700
H	-5.51751300	-4.57507000	0.42462200
H	-6.03456700	-3.90641300	2.75425600

H	-6.42616900	-1.52274600	3.34181200
H	-5.38264300	-2.84567100	-1.36431500
H	-5.50280900	-0.41739400	-2.01066600
H	-6.69610100	2.88141800	2.28020100
H	-6.57898500	4.76465500	0.66096300
H	-6.09060100	4.35626600	-1.73390200
H	-5.70311800	2.03268500	-2.54484000

47H (Charge = 1, Multiplicity = 2):

C	-7.40127000	0.04151800	0.71308100
C	-7.34417800	1.42228100	0.42291200
C	-6.14300500	2.05683900	0.18424100
C	-4.95058900	1.31572600	0.23377100
C	-4.98529600	-0.07315000	0.53277100
C	-6.24507100	-0.69274200	0.76267900
S	-3.48496000	2.17034800	-0.08931100
C	-2.23639700	0.99198400	0.09526300
C	-2.49912200	-0.36845200	0.41000600
C	-3.81335000	-0.85793000	0.56309200
C	-0.91456500	1.43199900	-0.08534200
C	0.12163200	0.53063200	0.04236700
C	-0.11829500	-0.82666100	0.34914400
C	-1.40364600	-1.26828100	0.52559700
C	-4.00776300	-1.56101200	-1.83830900
F	-5.16988500	-2.12441500	-2.06132900
F	-3.00784500	-2.34657700	-2.15494200
F	-3.91245900	-0.38880700	-2.42678300
H	-8.35975500	-0.43162000	0.89320300
H	-8.26221500	1.99919900	0.38457800
H	-6.11616100	3.11830200	-0.04047900
H	-6.25974800	-1.75633900	0.97957100
H	-3.92342600	-1.90888600	0.82820900
H	-0.71401900	2.47178600	-0.32293700
H	1.14095300	0.87497100	-0.09777800
H	0.71525700	-1.51353100	0.44051400
H	-1.61863300	-2.30718100	0.75621500

Coordinate of Products

CF3 (Charge = 0, Multiplicity = 2):

C	-3.06793400	0.05417900	0.00000000
F	-2.61141600	0.64474100	1.08619600
F	-2.61141600	0.64474100	-1.08619600
F	-4.38528600	0.01755800	0.00000000

IH (Charge = 1, Multiplicity = 1):

C	-2.11619200	0.66218800	0.55518500
C	-2.66562600	1.67754800	-0.22966700
N	-3.80119600	1.37321500	-0.89692100
C	-4.47146000	0.19948100	-0.89515500
C	-3.92771100	-0.82358300	-0.11630800
C	-2.75863000	-0.57094200	0.59347900
C	-2.14274300	3.06323100	-0.42131000
C	-5.70831200	0.14795000	-1.72957300
C	-4.50477200	-2.20249800	0.02188200
O	-3.97187200	-3.05723300	0.69074900
O	-5.63239100	-2.36813900	-0.65268400
C	-7.50763500	-3.63059300	-1.38749200
C	-6.24315500	-3.67760200	-0.56466700
C	-0.86417500	0.78366800	1.37455300
O	-0.41112700	-0.15023900	1.99470800
O	-0.33193900	1.99610100	1.34477300
C	1.30719000	3.61422200	1.93502800
C	0.88053100	2.17781600	2.11483300
H	-4.19882300	2.11956500	-1.46832700
H	-2.33193500	-1.36484100	1.19856400
H	-1.12102600	3.02542900	-0.80320300
H	-2.77208600	3.61659500	-1.11973800
H	-2.11631300	3.58512900	0.53731000
H	-5.87256900	1.10346600	-2.22834700
H	-5.62004600	-0.64302500	-2.47674400
H	-6.56953500	-0.08840600	-1.10183900
H	-8.00073700	-4.60470200	-1.34720200
H	-8.19630400	-2.87708300	-0.99704700
H	-7.28293200	-3.39869900	-2.43162200
H	-5.52968000	-4.41445200	-0.94247700
H	-6.44155200	-3.89350400	0.48821100
H	2.22283300	3.79223500	2.50390100
H	1.50546400	3.83109600	0.88237200
H	0.53486400	4.29664700	2.29859200
H	0.66240500	1.93732600	3.15842400
H	1.62996700	1.47335400	1.74515600

2H (Charge = 1, Multiplicity = 1):

C	-4.02017600	0.19679800	1.15000000
C	-4.30407400	1.29228900	0.33152100
N	-5.28144800	1.13419200	-0.58217300
C	-6.01206700	0.01993900	-0.78007000
C	-5.72678000	-1.07622200	0.03727000
C	-4.73003000	-0.99328500	1.00669300

C	-3.59030700	2.59345300	0.40440500
C	-7.06452600	0.01904500	-1.82951600
C	-6.48491300	-2.28330300	-0.13684400
N	-7.10097300	-3.24977500	-0.28375300
C	-2.98459800	0.32153200	2.13715600
N	-2.14882900	0.43241800	2.92732800
H	-5.48663100	1.93626500	-1.18340000
H	-4.50990200	-1.84489000	1.64161100
H	-4.06076200	3.33502800	-0.24056000
H	-3.58771700	2.95408300	1.43621200
H	-2.55055200	2.44962900	0.09367200
H	-7.09473800	0.96970500	-2.36213800
H	-6.86956100	-0.79155800	-2.53742900
H	-8.03593600	-0.16900000	-1.36202400

3H (Charge = 1, Multiplicity = 1):

C	-3.72271000	0.47931400	0.64702700
C	-4.26303200	1.48950400	-0.14849600
N	-5.38676200	1.18734800	-0.83603200
C	-6.06722100	0.01930100	-0.82959200
C	-5.54085300	-1.00928900	-0.04707900
C	-4.36392000	-0.75724800	0.65503800
C	-3.71872900	2.86533800	-0.35842000
C	-7.28490100	-0.02997200	-1.69441400
C	-6.11492000	-2.40608600	0.09404900
O	-5.36356400	-3.28451200	0.46383600
C	-7.56990800	-2.67301600	-0.16399900
C	-2.46948700	0.58934000	1.49268100
O	-1.88199400	-0.43837700	1.75958800
C	-2.01702600	1.91846400	2.02609500
H	-5.76031200	1.92709700	-1.43129200
H	-3.93137000	-1.56033900	1.24309300
H	-2.65807400	2.81628500	-0.61007000
H	-4.24796200	3.36733800	-1.16992500
H	-3.83102100	3.46005800	0.55162500
H	-7.37433200	0.88461400	-2.28181100
H	-7.22999300	-0.87962700	-2.37743800
H	-8.18250900	-0.13618200	-1.08099900
H	-7.81379300	-3.65067700	0.25182000
H	-8.19917200	-1.90292200	0.28880300
H	-7.76766000	-2.68717300	-1.23963400
H	-1.32057000	1.73593000	2.84476100
H	-1.49958100	2.48268800	1.24449100
H	-2.86343100	2.51501900	2.37489400

4H (Charge = 1, Multiplicity = 1):

C	-3.79430600	0.47555100	0.67930900
C	-4.31342200	1.46918900	-0.14784800
N	-5.41949100	1.15635200	-0.85827200
C	-6.09723400	-0.01216400	-0.83393900
C	-5.59526800	-1.01453300	-0.00762300
C	-4.42332500	-0.76586900	0.70048800
C	-3.75641600	2.84098900	-0.35425200

C	-7.29572200	-0.10458500	-1.72215100
C	-6.17884900	-2.40338400	0.11669200
O	-5.42613800	-3.36044500	0.22148500
N	-7.52151100	-2.49494400	0.11843800
C	-2.52828700	0.60197000	1.49619200
O	-1.77573000	-0.35742100	1.57898600
N	-2.31161800	1.78375500	2.10257800
H	-5.77563100	1.87622900	-1.48884000
H	-3.98907400	-1.56554200	1.29282000
H	-2.66698100	2.82224600	-0.32083400
H	-4.08270500	3.24435200	-1.31463700
H	-4.11450800	3.50956900	0.43534100
H	-7.21158400	0.60323600	-2.54886300
H	-7.40159100	-1.11347200	-2.12016500
H	-8.19923500	0.13969800	-1.15356000
H	-8.11506900	-1.68392100	0.22188300
H	-7.93427300	-3.40669800	0.26761800
H	-3.03265300	2.48615300	2.18779600
H	-1.50513900	1.86052700	2.70914900

5H (Charge = 1, Multiplicity = 1):

C	-2.05722400	0.84049900	0.46244300
C	-2.59082900	1.87256200	-0.29004900
N	-3.71296200	1.65194700	-0.99077300
C	-4.36446800	0.47998200	-1.01052900
C	-3.86418200	-0.57666400	-0.26950500
C	-2.70022400	-0.39448000	0.47237700
C	-4.54278700	-1.91313900	-0.24921300
O	-4.11630800	-2.84840500	0.38410800
O	-5.63588500	-1.92296700	-0.99724800
C	-7.55963200	-2.96258700	-1.93851500
C	-6.36273900	-3.17538300	-1.04479700
C	-0.80413800	1.01802700	1.26587700
O	-0.32216400	0.12629500	1.92189600
O	-0.31746600	2.24530300	1.15865300
C	1.27188300	3.95127900	1.64059100
C	0.89755800	2.51311500	1.90121500
H	-2.16077800	2.86418300	-0.35427000
H	-4.09391300	2.42296200	-1.54171600
H	-5.26041800	0.42693800	-1.61637800
H	-2.29443800	-1.21470500	1.05756300
H	-8.13245900	-3.89096300	-1.99861700
H	-8.20868900	-2.18001000	-1.53818000
H	-7.24583800	-2.68270400	-2.94705800
H	-5.68971200	-3.94537600	-1.43050300
H	-6.64959900	-3.44209000	-0.02441600
H	2.18694300	4.18893100	2.18819600
H	1.45147800	4.11884200	0.57590000
H	0.48084800	4.62522800	1.97814100
H	0.69945800	2.32179100	2.95886400
H	1.66650400	1.81590400	1.55888800

6H (Charge = 1, Multiplicity = 1):

C	-2.40189500	0.66773800	0.96217800
C	-2.95434400	1.67861400	0.17605100
N	-4.07135900	1.38918400	-0.55313600
C	-4.73708700	0.19998300	-0.47787700
C	-4.19033300	-0.81162500	0.31117000
C	-3.03435000	-0.56420100	1.03650900
C	-2.42958600	3.08024600	0.14258000
C	-6.04760200	0.07685400	-1.19012400
C	-4.58438300	2.42099100	-1.48606500
C	-4.76420000	-2.19461900	0.44000900
O	-4.66029500	-2.84075600	1.45592100
O	-5.31491200	-2.63398700	-0.68377400
C	-6.49616300	-4.23895000	-1.98347000
C	-5.87166100	-3.97018200	-0.63607400
C	-1.13064100	0.80185000	1.75269800
O	-0.95142500	0.20407700	2.78754400
O	-0.22928400	1.57021100	1.15549300
C	1.88719500	2.64738800	1.01745400
C	1.03386800	1.72015100	1.84791400
H	-2.61830900	-1.34331500	1.66770200
H	-1.80729800	3.26185400	1.01433900
H	-1.82272500	3.24830700	-0.75336900
H	-3.25401600	3.79477300	0.14593700
H	-6.61798900	1.00232700	-1.09909400
H	-5.89374200	-0.13765900	-2.25304000
H	-6.62762300	-0.73460000	-0.76019900
H	-3.74781000	3.00476000	-1.85653500
H	-5.05864000	1.92871300	-2.32894900
H	-5.29909900	3.06295300	-0.96765400
H	-6.92341500	-5.24451000	-1.98823600
H	-7.29456700	-3.52202300	-2.19107400
H	-5.74819700	-4.17617300	-2.77755400
H	-5.06247600	-4.66847900	-0.40741300
H	-6.60354600	-4.00942000	0.17469400
H	2.85361800	2.78405700	1.50841300
H	2.05928900	2.22904700	0.02279300
H	1.40973700	3.62493800	0.91298200
H	0.83418600	2.12199900	2.84459800
H	1.48340900	0.72976100	1.95630200

7H (Charge = 1, Multiplicity = 1):

C	-2.05899300	0.56950300	0.61864600
C	-2.62697100	1.59608400	-0.11895000
N	-3.77293900	1.39365200	-0.79011300
C	-4.40007400	0.20237200	-0.76923900
C	-3.87114700	-0.85193400	-0.04761800
C	-2.68494900	-0.66999600	0.65728100
C	-4.36943500	2.48522300	-1.59023400
C	-4.54595200	-2.19012100	-0.00877600
O	-4.10223100	-3.12243300	0.61731000
O	-5.65561800	-2.20797400	-0.73249600
C	-7.59048200	-3.26377900	-1.63231700
C	-6.37724700	-3.46383200	-0.75789700

C	-0.78320900	0.76963100	1.37993700
O	-0.26682500	-0.11071600	2.02524300
O	-0.31737200	2.00355100	1.25180600
C	1.26357500	3.73354900	1.66957500
C	0.91502100	2.29363000	1.95564000
H	-2.18832400	2.58406300	-0.18766400
H	-5.31780900	0.12955100	-1.34114100
H	-2.25578700	-1.48646300	1.23002800
H	-5.40806100	2.60406800	-1.28524400
H	-3.81130100	3.39934200	-1.40322400
H	-4.30867100	2.20937100	-2.64268600
H	-8.16035700	-4.19497900	-1.67422200
H	-8.23579500	-2.48032700	-1.22766100
H	-7.29548000	-2.99166300	-2.64863200
H	-5.70762500	-4.23397100	-1.14919100
H	-6.64532600	-3.72417400	0.26924900
H	2.19076000	3.98856000	2.18822400
H	1.41041100	3.89191900	0.59844300
H	0.47394600	4.40122300	2.02260700
H	0.75027400	2.11120900	3.02063400
H	1.68266800	1.60244900	1.59855600

8H (Charge = 1, Multiplicity = 1):

C	-4.96559100	0.75159700	0.77043700
C	-5.34380900	1.75951500	-0.10555000
N	-6.38884200	1.54821900	-0.91493200
C	-7.10620800	0.41829500	-0.93756100
C	-6.75569100	-0.61055200	-0.07454600
C	-5.67422300	-0.45113300	0.79410800
C	-7.51626300	-1.83052000	-0.08630300
N	-8.12450200	-2.81208400	-0.09483200
C	-3.84850300	0.96260100	1.65070300
N	-2.95401000	1.12664500	2.36237100
H	-4.84211600	2.71669800	-0.17702300
H	-6.65934200	2.29936000	-1.55469000
H	-7.93168200	0.36640700	-1.63753700
H	-5.38964100	-1.24619100	1.47492800

9H (Charge = 1, Multiplicity = 1):

C	-4.14039400	0.89814800	0.31966300
C	-4.72867100	1.73875400	-0.60947900
N	-5.83446900	1.33151100	-1.25061700
C	-6.43175300	0.14901300	-1.03797000
C	-5.88189700	-0.72684600	-0.11774900
C	-4.71013900	-0.35424800	0.53759400
C	-6.45175300	-2.09821200	0.16127600
O	-5.71870800	-2.97309400	0.59609700
N	-7.75776600	-2.26423700	-0.11219800
C	-2.86914700	1.24556200	1.05879700
O	-2.16132000	0.34646300	1.48566000
N	-2.59236400	2.55643700	1.17984800
H	-4.34941200	2.71441400	-0.88930000
H	-6.23945800	1.95418300	-1.95057900

H	-7.31373300	-0.05167200	-1.63458000
H	-4.23835100	-1.04643000	1.22849600
H	-8.37924100	-1.48640200	-0.28326800
H	-8.17479700	-3.16156900	0.09804100
H	-3.28341200	3.27312700	1.00806200
H	-1.77071200	2.81728500	1.70939500

10H (Charge = 1, Multiplicity = 1):

C	-2.13856500	1.98719000	1.04721300
C	-2.70620800	2.95261500	0.23810700
N	-3.80401800	2.65094400	-0.47649900
C	-4.39974000	1.45083000	-0.45519900
C	-3.86362500	0.45446900	0.34133500
C	-2.72287900	0.72574900	1.09770200
C	-4.48183300	-0.90827600	0.40806600
O	-4.01217800	-1.80729200	1.06401900
O	-5.58292000	-0.99037600	-0.32673700
C	-7.49480400	-2.12933000	-1.17134700
C	-6.25443900	-2.27295600	-0.32395500
H	-1.25419600	2.22543200	1.62392900
H	-2.32505000	3.96024600	0.13296300
H	-4.20737700	3.37708600	-1.06908900
H	-5.27989000	1.32814900	-1.07317200
H	-2.30441700	-0.05886500	1.71992000
H	-8.02764400	-3.08287700	-1.19365200
H	-8.16155200	-1.36931400	-0.75675700
H	-7.23513500	-1.85308200	-2.19617800
H	-5.56448800	-3.02066100	-0.72386900
H	-6.48886200	-2.53447600	0.71102900

11H (Charge = 1, Multiplicity = 1):

C	-4.90215900	1.06119600	0.54832400
C	-5.57963500	1.81975700	-0.38735700
N	-6.73694400	1.36166600	-0.89556500
C	-7.29296700	0.19526400	-0.55131300
C	-6.64382900	-0.59488900	0.38597300
C	-5.43516400	-0.16038100	0.94306200
C	-7.22613800	-1.85207600	0.77101900
N	-7.68960400	-2.86251000	1.08551400
H	-3.97059100	1.42612400	0.96068800
H	-5.23922900	2.78019500	-0.75235200
H	-7.22058300	1.93626100	-1.58771800
H	-8.22793100	-0.07336700	-1.02722500
H	-4.92757100	-0.77801200	1.67608600

12H (Charge = 1, Multiplicity = 1):

C	-3.72457900	1.38018700	0.80951100
C	-4.28844600	2.32900800	-0.02238400
N	-5.40772200	2.02566400	-0.70007200
C	-6.02853300	0.83894300	-0.62057700
C	-5.50204900	-0.14478500	0.19874400
C	-4.33685800	0.13695400	0.91801900
C	-6.14745500	-1.50304700	0.33776200

O	-5.62400500	-2.32131500	1.06356800
C	-7.40892500	-1.77513600	-0.42848600
H	-2.82250900	1.61905300	1.35813900
H	-3.88786000	3.32329300	-0.17329300
H	-5.80909600	2.73809300	-1.30996100
H	-6.92412900	0.72706600	-1.21920100
H	-3.92294600	-0.63369400	1.56051100
H	-7.74466000	-2.78922400	-0.21552500
H	-8.18523300	-1.05828000	-0.14226000
H	-7.22955700	-1.66129900	-1.50235700

13H (Charge = 1, Multiplicity = 1):

C	-4.26228300	1.49543800	0.47646400
C	-4.91768200	2.22187300	-0.49968700
N	-5.99045400	1.68665900	-1.10445400
C	-6.48496000	0.47471900	-0.80975500
C	-5.87043300	-0.28454300	0.16946800
C	-4.73645800	0.22939900	0.80231000
C	-6.33817300	-1.66978900	0.54553500
O	-5.55117800	-2.45064100	1.05924300
N	-7.62146900	-1.96197300	0.26377500
H	-3.39327700	1.91809500	0.96399500
H	-4.62228500	3.21085800	-0.82560300
H	-6.45175100	2.22805600	-1.83603000
H	-7.34516600	0.15581700	-1.38548200
H	-4.23882800	-0.37742900	1.55174400
H	-8.30215500	-1.25485100	0.02519200
H	-7.96909400	-2.87093900	0.53984000

14H (Charge = 1, Multiplicity = 1):

C	-4.50181100	0.92990700	1.25669900
C	-5.07115200	1.83958700	0.38812100
N	-6.00557700	1.44548800	-0.49966300
C	-6.42225300	0.16847600	-0.55913700
C	-5.89157600	-0.78293900	0.29584700
C	-4.90590200	-0.39869300	1.20290600
C	-6.55009800	2.44520800	-1.44141700
C	-6.29405800	-2.23752500	0.24965600
O	-5.51985300	-3.08698100	0.66451500
N	-7.50301100	-2.50914700	-0.27723200
H	-3.74965500	1.26783400	1.95810200
H	-4.80388900	2.88945300	0.36573200
H	-7.16487700	-0.05428300	-1.31651700
H	-4.47069600	-1.14687800	1.85688500
H	-6.83761800	3.32973900	-0.87485600
H	-5.77567500	2.69338600	-2.16703900
H	-7.41665200	2.01899000	-1.94109900
H	-8.20630000	-1.79760600	-0.41677300
H	-7.80800400	-3.47369800	-0.27533200

15H (Charge = 1, Multiplicity = 1):

C	-5.15878700	0.41448700	1.14728700
C	-5.34519100	1.57213500	0.41741700

N	-6.21501500	1.56882200	-0.60602100
C	-6.93020500	0.49172500	-0.97007800
C	-6.77589500	-0.68810300	-0.26867300
C	-5.88142500	-0.72540600	0.79958200
H	-4.45850300	0.41260800	1.97294900
H	-4.83030400	2.50416600	0.61170100
H	-6.34143400	2.43182400	-1.13412800
H	-7.59861100	0.61694200	-1.81195200
H	-7.34928700	-1.55924100	-0.55902200
H	-5.74728000	-1.64346200	1.36144500

16H (Charge = 1, Multiplicity = 1):

C	-2.79496700	1.41887300	-0.18186400
C	-2.23719900	0.13142700	0.01849500
C	-3.02345400	-0.99442100	0.00322000
C	-4.40659200	-0.84313700	-0.21630700
C	-4.98773400	0.43209600	-0.41720000
C	-4.14097500	1.57002100	-0.39526700
N	-5.23468000	-1.93452500	-0.24079900
C	-6.54386000	-1.86470500	-0.44044800
C	-7.15942900	-0.62606400	-0.64113600
C	-6.38423900	0.51170700	-0.62975900
H	-2.14559500	2.28725500	-0.16464200
H	-1.16998400	0.03437500	0.18706700
H	-2.60986800	-1.98639000	0.15398600
H	-4.58337400	2.54889100	-0.55024000
H	-4.81387200	-2.85299300	-0.09942300
H	-7.08351500	-2.80354600	-0.43685100
H	-8.22863200	-0.58867800	-0.80302800
H	-6.83435700	1.48798200	-0.78462300

17H (Charge = 1, Multiplicity = 1):

C	-0.71207400	1.23045500	-0.02398900
C	-0.22996400	-0.08955400	0.15415000
C	-1.08134700	-1.16857400	0.13463700
C	-2.45303700	-0.93158700	-0.06616900
C	-2.96045800	0.37801000	-0.24166300
C	-2.04935700	1.46454200	-0.21919000
N	-3.34754600	-1.97161700	-0.10335800
C	-4.64676700	-1.82093300	-0.28790300
C	-5.19807300	-0.54140200	-0.44552700
C	-4.35119100	0.54672300	-0.43194200
C	-6.68704100	-0.48885900	-0.67134300
O	-7.28334000	-1.50624000	-0.99970000
N	-7.27533900	0.70891600	-0.50832200
H	-0.01218800	2.05851300	-0.00407600
H	0.83159600	-0.25123300	0.30805500
H	-0.72490400	-2.18472300	0.26788000
H	-2.43490400	2.46968400	-0.35563000
H	-2.98212700	-2.91767100	0.01307400
H	-5.25792800	-2.71509200	-0.31211900
H	-4.72681500	1.55564300	-0.58038400
H	-6.80858200	1.49410800	-0.07794800

H -8.27855400 0.76212100 -0.62367000

18H (Charge = 1, Multiplicity = 1):

C -1.18205300 2.28869600 -0.33853600
C -0.36805700 1.13943300 -0.22867500
C -0.91183200 -0.12276000 -0.14973100
C -2.31330000 -0.26331100 -0.18133500
C -3.14575700 0.87966800 -0.28856800
C -2.54714700 2.16167000 -0.36801300
N -2.91677500 -1.50888900 -0.11242900
C -4.23318600 -1.64151800 -0.14521500
C -5.09839500 -0.54105900 -0.24199200
C -4.54950200 0.71724100 -0.31752100
C -2.07436900 -2.71410500 -0.00679300
C -6.56720300 -0.88131900 -0.28897500
O -6.91099100 -2.05401000 -0.37400100
N -7.43138200 0.14532000 -0.24630600
H -0.72153400 3.26838400 -0.39890300
H 0.71074700 1.25058200 -0.20586600
H -0.26724400 -0.98812300 -0.06717000
H -3.19501200 3.02841000 -0.45043700
H -4.63450400 -2.64717600 -0.09751000
H -5.15874800 1.61218100 -0.40885400
H -2.72553300 -3.58363500 0.02583200
H -1.42181100 -2.76785100 -0.87850800
H -1.48335800 -2.65546900 0.90732700
H -7.15701200 1.10278100 -0.08899600
H -8.41944900 -0.06870300 -0.26134600

19H (Charge = 1, Multiplicity = 1):

C -1.54202700 1.61749800 -0.27965900
C -0.88779300 0.37754200 -0.07697700
C -1.59233100 -0.80173700 -0.01150000
C -2.98913900 -0.74987100 -0.15054500
C -3.66761300 0.47860600 -0.35321900
C -2.90544400 1.67285000 -0.41556900
N -3.74082200 -1.89694300 -0.09475800
C -5.05393900 -1.93209100 -0.21844500
C -5.75966200 -0.73428100 -0.42025700
C -5.07016600 0.46432700 -0.48634800
C -7.18869300 -0.77962500 -0.55496100
N -8.33871900 -0.81252200 -0.66537400
H -0.95349100 2.52682800 -0.32620500
H 0.19155900 0.35835000 0.02868900
H -1.10221900 -1.75754300 0.14229300
H -3.42395900 2.61303300 -0.57169900
H -3.24983300 -2.78090800 0.05144000
H -5.53642800 -2.90007800 -0.15782000
H -5.60498500 1.39644400 -0.64312700

20H (Charge = 1, Multiplicity = 1):

C 1.23931700 1.59110300 -0.21627300
C 1.97390000 0.38266900 -0.13637800

C	1.34041000	-0.83645000	-0.08012600
C	-0.06492500	-0.85814700	-0.10377700
C	-0.82301200	0.33621400	-0.18401200
C	-0.13202100	1.57350300	-0.24040600
N	-0.74784100	-2.04794100	-0.04941700
C	-2.06452000	-2.14495200	-0.06810700
C	-2.85114600	-0.98829600	-0.14406800
C	-2.23234400	0.24349600	-0.20210100
C	-4.33293000	-1.17634400	-0.16076100
O	-4.85537100	-2.26755300	-0.14302900
O	-4.98213700	-0.02086200	-0.19507400
C	-6.95908700	1.30442800	-0.21814500
C	-6.42657000	-0.10757800	-0.21436200
H	1.77242800	2.53431100	-0.25803900
H	3.05785600	0.42048300	-0.11882600
H	1.89264800	-1.76864200	-0.01876800
H	-0.71068800	2.48937800	-0.30066500
H	-0.20091300	-2.90872300	0.00765300
H	-2.49411500	-3.13865700	-0.02256700
H	-2.82329500	1.15267400	-0.26248700
H	-8.05125400	1.27712600	-0.23335300
H	-6.63823800	1.84195500	0.67748000
H	-6.61345200	1.84762700	-1.10100900
H	-6.72459800	-0.66403000	-1.10690900
H	-6.74859600	-0.66768900	0.66724200

21H (Charge = 1, Multiplicity = 1):

C	-0.06980100	0.40896300	0.98045300
C	-0.04429700	1.16408700	-0.22610200
C	-1.18130200	1.39042000	-0.95570400
C	-2.40456400	0.85584800	-0.48920800
C	-2.45462200	0.09764600	0.71714100
C	-1.24438100	-0.11182900	1.44251500
N	-3.55361200	1.05315800	-1.17828600
C	-4.76435000	0.57990900	-0.79827000
C	-4.85349400	-0.18081200	0.40400800
C	-3.68722200	-0.40710700	1.13894800
C	-5.91597400	0.83588700	-1.57742000
C	-7.12034600	0.33994500	-1.15355000
C	-7.23388600	-0.42164600	0.04382200
C	-6.12931800	-0.67746400	0.80475300
H	0.85280500	0.25228500	1.52789400
H	0.89962500	1.56960300	-0.57504900
H	-1.16796800	1.96584300	-1.87560100
H	-1.28832600	-0.69016300	2.35977700
H	-3.50478000	1.59459600	-2.04167600
H	-3.73952800	-0.98676700	2.05748100
H	-5.82338000	1.41784700	-2.48859800
H	-8.01043800	0.53207800	-1.74361500
H	-8.20598600	-0.79602700	0.34416700
H	-6.19103100	-1.25606300	1.72082800

22H (Charge = 1, Multiplicity = 1):

C	-0.13063700	0.42452800	1.37852100
C	-0.09926600	1.18408300	0.18028400
C	-1.21214600	1.35800100	-0.60283000
C	-2.44319400	0.76982400	-0.21189500
C	-2.49228900	0.03437000	1.01183600
C	-1.30672200	-0.13332000	1.78616000
N	-3.57950500	0.90007000	-0.96585700
C	-4.79739000	0.45708500	-0.52189800
C	-4.87196700	-0.28272900	0.69869900
C	-3.70801200	-0.49924300	1.43111300
C	-5.99918800	0.71987400	-1.23001200
C	-7.18947100	0.23706600	-0.74850200
C	-7.26743200	-0.52910300	0.44335800
C	-6.12974200	-0.77789400	1.15311700
C	-3.48234000	1.53836400	-2.29111700
H	0.77354800	0.30545800	1.96444600
H	0.83100100	1.65134400	-0.12600100
H	-1.14159600	1.96999400	-1.49083700
H	-1.37834500	-0.70658000	2.70499600
H	-3.75254800	-1.07465700	2.35248900
H	-6.00111200	1.32220900	-2.12727100
H	-8.09989500	0.45819100	-1.29611000
H	-8.22782800	-0.89762100	0.78512600
H	-6.14652200	-1.34493500	2.07848300
H	-2.51881300	1.29673600	-2.73039200
H	-4.24739500	1.12994600	-2.94340300
H	-3.59879000	2.61985500	-2.19727700

23H (Charge = 1, Multiplicity = 1):

N	-0.00389900	-0.99943000	0.32366000
C	0.17967800	0.28325400	-0.15627200
N	-0.97423100	1.02873700	-0.41768900
C	-2.23536300	0.59097400	-0.20698100
C	-2.41496100	-0.70486300	0.33729400
C	-1.24099100	-1.56122100	0.61694000
N	-3.28509900	1.36176400	-0.52049800
C	-4.58399500	0.96911600	-0.18806000
C	-4.79432700	-0.32307100	0.35478800
C	-3.67818900	-1.15641100	0.59260600
C	-5.67945900	1.83160000	-0.36604500
C	-6.94549000	1.38979500	-0.03648100
C	-7.17157400	0.09640200	0.47146500
C	-6.10600600	-0.74678100	0.66960800
C	-3.05872200	2.63345800	-1.23085600
O	-1.35358000	-2.68177400	1.06874000
O	1.27179800	0.76316200	-0.35261000
C	1.21641600	-1.77180000	0.57057100
H	-0.77785000	1.98133200	-0.71042400
H	-3.81702200	-2.15393700	0.99987300
H	-5.54994900	2.84284300	-0.72650500
H	-7.78310200	2.06654200	-0.16836800
H	-8.17901800	-0.22110100	0.71494600
H	-6.23869900	-1.74425400	1.07623300

H	-3.93088300	2.85815800	-1.83615000
H	-2.86918000	3.43611400	-0.51595600
H	-2.21806200	2.51242200	-1.91253400
H	1.78691500	-1.31216500	1.37893500
H	0.91995500	-2.77960900	0.84719700
H	1.81999600	-1.79047300	-0.33652400

24H (Charge = 1, Multiplicity = 1):

N	0.00245700	-1.16569700	0.24250700
C	0.17043000	0.18080400	-0.02845800
N	-0.98331000	0.99004700	-0.08859900
C	-2.23177300	0.45190400	-0.01960200
C	-2.38527900	-0.87672500	0.45738900
C	-1.19773900	-1.73746300	0.63383400
N	-3.31624200	1.15216500	-0.39821600
C	-4.60046100	0.71630600	-0.06107400
C	-4.77369400	-0.56592300	0.51156600
C	-3.63196000	-1.37372600	0.70992600
C	-5.72050900	1.53245000	-0.29426500
C	-6.97443900	1.06566500	0.04686700
C	-7.16123900	-0.21230400	0.60849300
C	-6.07266900	-1.01855800	0.83669000
C	-3.21184700	2.28220300	-1.34969500
O	-1.27152300	-2.87904700	1.03986400
O	1.26422600	0.67274800	-0.18646200
C	1.22119400	-1.97720700	0.29040100
C	-0.71485600	2.43494400	0.07092100
H	-3.73369500	-2.38931000	1.08192900
H	-5.61194500	2.52581900	-0.70980200
H	-7.83359700	1.70671200	-0.12026600
H	-8.15970300	-0.55095000	0.86059300
H	-6.17969600	-2.00806900	1.26934000
H	-3.97952200	2.13320900	-2.10735200
H	-3.35777500	3.23860200	-0.84788300
H	-2.24328900	2.24412400	-1.83806600
H	1.84581900	-1.72259700	-0.56363900
H	1.76837800	-1.78320300	1.21530600
H	0.92642900	-3.02238900	0.24626200
H	0.10790800	2.53371600	0.77629600
H	-0.43589300	2.89795000	-0.87497200
H	-1.59971900	2.90922400	0.48865600

25H (Charge = 1, Multiplicity = 1):

C	-2.26603300	0.88395800	0.95418200
C	-2.55454300	2.20335200	1.37757900
C	-3.82816200	2.69124100	1.26263600
C	-4.84634500	1.86313800	0.72256000
C	-4.56480000	0.52562400	0.30387400
C	-3.23466700	0.05834000	0.43181000
C	-6.14850500	2.36292700	0.59068500
N	-7.10043800	1.60235800	0.07573600
C	-6.89193900	0.32416000	-0.34422800
C	-5.65103700	-0.23810600	-0.23814000

C	-5.49578200	-1.66827800	-0.66722800
O	-4.61675400	-2.40259300	-0.27914800
O	-6.45756500	-2.02604600	-1.51419300
C	-7.09693700	-4.28895200	-0.86917300
C	-6.46835900	-3.41244500	-1.93117100
H	-1.25001600	0.51304300	1.04351900
H	-1.76332900	2.82195600	1.78620800
H	-4.08297200	3.70051300	1.56980600
H	-2.98716100	-0.94626900	0.12010700
H	-6.42301500	3.36703200	0.89441000
H	-8.04049900	1.98784500	-0.00889800
H	-7.75414400	-0.19183200	-0.74304800
H	-7.15071900	-5.31728900	-1.23595700
H	-6.50250100	-4.27996000	0.04724900
H	-8.11049900	-3.94920900	-0.64197900
H	-7.05396100	-3.40958800	-2.85060800
H	-5.44359100	-3.71473900	-2.15505200

26H (Charge = 1, Multiplicity = 1):

C	-2.46887300	-0.18011800	0.15220900
C	-2.53684100	1.21495900	-0.08172900
C	-3.74993700	1.81570900	-0.28731500
C	-4.93039400	1.02896200	-0.26088500
C	-4.86918000	-0.37672600	-0.02080800
C	-3.59788300	-0.96447800	0.18521700
C	-6.18016400	1.63041000	-0.47102000
N	-7.27741800	0.89420000	-0.45679700
C	-7.27542000	-0.45460900	-0.24687900
C	-6.09869800	-1.11093100	-0.02879800
C	-6.13217800	-2.59179200	0.27010000
O	-5.44728000	-3.06612100	1.16577700
N	-6.98291600	-3.30757100	-0.48801800
H	-1.49897800	-0.64107600	0.30937600
H	-1.62479700	1.80114400	-0.09927800
H	-3.83471600	2.88160500	-0.47378100
H	-3.52680300	-2.02745400	0.37394100
H	-6.29597400	2.69363400	-0.64999700
H	-8.17509300	1.35373800	-0.60548100
H	-8.24698700	-0.93167800	-0.24914100
H	-7.42866500	-2.92288000	-1.30879000
H	-7.04710400	-4.30430200	-0.32735300

27H (Charge = 1, Multiplicity = 1):

C	-1.29194900	-0.30281600	0.32144000
C	-1.39342100	1.09946400	0.15718500
C	-2.61603000	1.67775500	-0.06264300
C	-3.77251800	0.85926700	-0.11899600
C	-3.67729400	-0.55026500	0.05541000
C	-2.39957700	-1.11713900	0.27500600
C	-5.03204100	1.44046600	-0.34687300
N	-6.12555800	0.70009100	-0.41015300
C	-6.07210900	-0.66243500	-0.25779100
C	-4.89093400	-1.30396800	-0.02956400

C	-7.44641700	1.31420000	-0.63608100
C	-4.90532700	-2.79612400	0.20912600
O	-4.24136600	-3.29063800	1.10960400
N	-5.71519700	-3.49874800	-0.60406300
H	-0.31491000	-0.74487100	0.48828700
H	-0.49891600	1.71080900	0.20252100
H	-2.72299800	2.74920500	-0.19835900
H	-2.30670100	-2.18662900	0.41127100
H	-5.14941900	2.51106000	-0.47746800
H	-7.02678200	-1.17210100	-0.31189200
H	-7.87694400	0.88463100	-1.54040200
H	-8.07964600	1.09548100	0.22377300
H	-7.31854900	2.38819400	-0.74954500
H	-6.13797400	-3.09165200	-1.42613800
H	-5.76235800	-4.50222000	-0.48519100

28H (Charge = 1, Multiplicity = 1):

C	-2.48401200	-0.69728600	-0.22772300
C	-2.54184500	0.70312300	-0.43306700
C	-3.75230100	1.33872000	-0.52371900
C	-4.94518500	0.57936800	-0.41036200
C	-4.88462500	-0.82934900	-0.20391900
C	-3.62554800	-1.45671800	-0.11356800
C	-6.20019300	1.19746000	-0.49931600
N	-7.30787600	0.47795900	-0.39233400
C	-7.31860300	-0.86821000	-0.19555500
C	-6.12709900	-1.53169300	-0.09969600
C	-6.13972900	-2.95286800	0.10733800
N	-6.12712200	-4.09679100	0.27318200
H	-1.51518300	-1.18091700	-0.15939100
H	-1.62044400	1.26811300	-0.51792700
H	-3.82414900	2.40990500	-0.68124700
H	-3.56676600	-2.52883700	0.04344000
H	-6.31730400	2.26424900	-0.65541300
H	-8.20738900	0.95522700	-0.45919400
H	-8.28721100	-1.34459300	-0.12472200

29H (Charge = 1, Multiplicity = 1):

C	-6.89796000	1.78712000	-0.34636200
C	-6.03563500	2.89799900	-0.43723200
C	-4.67520400	2.70269300	-0.44781200
C	-4.15969900	1.38964800	-0.36374300
C	-5.02109100	0.26550700	-0.26782200
C	-6.40935600	0.49811400	-0.26422500
C	-2.75919100	1.18640300	-0.37847500
N	-2.25876800	-0.02056800	-0.30138700
C	-3.02478000	-1.17496600	-0.19873800
C	-4.42829000	-1.05642100	-0.17671100
C	-2.37531100	-2.41560100	-0.11866800
C	-3.13720400	-3.55825200	-0.01275800
C	-4.54117700	-3.47060900	0.01568200
C	-5.17473900	-2.24819300	-0.06407500
H	-7.97128700	1.94750200	-0.34063300

H	-6.44756000	3.89896700	-0.49951900
H	-3.98335900	3.53622300	-0.51912200
H	-7.10465700	-0.33004200	-0.19793600
H	-2.05820900	2.01099800	-0.45445400
H	-1.24446800	-0.13052300	-0.31978200
H	-1.29059500	-2.45228200	-0.14116000
H	-2.65239900	-4.52619700	0.05000500
H	-5.13276000	-4.37560300	0.10163800
H	-6.25725100	-2.20668900	-0.03822600

30H (Charge = 1, Multiplicity = 1):

C	-7.03948800	1.62746000	0.00894500
C	-6.24939000	2.78232500	-0.15729100
C	-4.88719100	2.65944700	-0.29596100
C	-4.30071000	1.37436400	-0.27047900
C	-5.08596000	0.21063800	-0.10492500
C	-6.47790700	0.36590300	0.03583000
C	-2.89898100	1.24661400	-0.41631400
N	-2.28953700	0.08540900	-0.40921900
C	-3.00093600	-1.11579200	-0.24879200
C	-4.40456000	-1.06968400	-0.09280200
C	-2.31317900	-2.34140200	-0.24399700
C	-3.01968500	-3.51518400	-0.08300800
C	-4.41379300	-3.49062700	0.07441300
C	-5.09082900	-2.29008200	0.06881700
C	-0.82586800	0.04197900	-0.57130600
H	-8.11430200	1.73085500	0.11805100
H	-6.71752500	3.76012100	-0.17524900
H	-4.24969500	3.52852100	-0.42580500
H	-7.11853900	-0.49800300	0.16460100
H	-2.27904800	2.12842000	-0.54113700
H	-1.23866800	-2.37527300	-0.36499300
H	-2.48789300	-4.46025800	-0.07878200
H	-4.96113100	-4.41835700	0.20093500
H	-6.16726800	-2.28484600	0.19145500
H	-0.46539200	1.06208800	-0.67751600
H	-0.38257200	-0.42075100	0.31053500
H	-0.58294800	-0.53370600	-1.46473200

31H (Charge = 1, Multiplicity = 1):

C	-0.69124800	-0.91909200	0.35733700
C	-0.26597700	0.40549500	0.23405300
C	-1.18620400	1.43964300	0.12590000
C	-2.55620300	1.14147200	0.14250100
C	-2.99564100	-0.20338800	0.26651000
C	-2.05122600	-1.25217700	0.37624900
C	-3.54389300	2.15378000	0.03727200
N	-4.82030400	1.85354400	0.05401300
C	-5.32171700	0.55936200	0.17125300
C	-4.38509300	-0.49046000	0.28098600
C	-6.69003600	0.31465100	0.17848000
C	-7.12767100	-1.00257100	0.29998100
C	-6.22580200	-2.05825700	0.41209100

C	-4.84524800	-1.82607700	0.40447500
C	-3.86348600	-2.87691700	0.51615000
C	-2.53471200	-2.60495900	0.50262800
H	0.04366000	-1.71482500	0.44171100
H	0.79546300	0.62666000	0.22262400
H	-0.86259700	2.47126300	0.03053500
H	-3.28480700	3.20287100	-0.05994100
H	-5.49675400	2.61346300	-0.02551400
H	-7.39085700	1.13858200	0.09066900
H	-8.19297600	-1.20586000	0.30704600
H	-6.59022700	-3.07653700	0.50672300
H	-4.21869900	-3.89838300	0.61229100
H	-1.80401600	-3.40358300	0.58793000

32H (Charge = 1, Multiplicity = 1):

C	-6.72204800	0.44376800	0.38113400
C	-7.07135600	-0.79956900	-0.21520400
C	-6.14536700	-1.78573000	-0.51082600
C	-4.76760100	-1.57854100	-0.21764300
C	-4.45459100	-0.35506500	0.36560700
C	-5.39034900	0.63697800	0.66330900
C	-3.65787300	-2.43762100	-0.43295700
C	-2.37337900	-2.04067400	-0.07187700
C	-2.09648600	-0.78802600	0.51759400
C	-3.16762500	0.06990300	0.73875300
C	-3.35907000	1.38544700	1.28775500
N	-4.64366200	1.69008000	1.23402400
H	-7.48115800	1.18815200	0.59475000
H	-8.11647600	-0.97375400	-0.44561700
H	-6.46968000	-2.71611600	-0.96642600
H	-3.81013500	-3.41421600	-0.88348800
H	-1.54806800	-2.72079300	-0.24994600
H	-1.07867800	-0.52070600	0.78205200
H	-2.63583500	2.07865100	1.69795600
H	-5.03510800	2.56808200	1.56830000

33H (Charge = 1, Multiplicity = 1):

C	-4.95346200	2.63756900	1.35419000
C	-5.15191200	3.19944700	0.08582100
C	-5.83636800	2.49428500	-0.88622300
C	-6.32560700	1.21817800	-0.59085700
C	-6.12538700	0.65272100	0.67835300
C	-5.43428800	1.37437400	1.65531900
N	-7.02144300	0.49329000	-1.55911700
C	-7.50874400	-0.71101400	-1.34321500
C	-7.33692300	-1.31901200	-0.10408800
N	-6.63893500	-0.63207700	0.90343400
C	-7.72077200	-2.55940500	0.41131800
C	-7.25177100	-2.61251200	1.72261000
C	-6.58915200	-1.41501300	2.00008900
H	-4.41737300	3.19478200	2.11448700
H	-4.76976400	4.18933200	-0.13635700
H	-6.00532100	2.90627500	-1.87614700

H	-5.27853200	0.94901500	2.63994600
H	-7.15331900	0.92357000	-2.47246300
H	-8.03733000	-1.20115900	-2.15214700
H	-8.27448200	-3.31283200	-0.13027000
H	-7.36725100	-3.42771300	2.42190000
H	-6.09425000	-1.09418000	2.90454300

34H (Charge = 1, Multiplicity = 1):

C	-7.12095500	-0.89686900	-0.39634400
C	-6.27689700	-1.98125000	-0.71562000
C	-4.91397700	-1.94357600	-0.47405900
C	-4.42300400	-0.77202500	0.10330600
C	-5.26049700	0.30352100	0.42083300
C	-6.63384100	0.26558600	0.17710800
N	-3.14449700	-0.38471600	0.47910800
C	-3.18672400	0.83882400	0.99132300
N	-4.43902100	1.27770200	0.97036300
H	-8.18186100	-0.97750500	-0.60677000
H	-6.70951100	-2.86919300	-1.16357200
H	-4.25825200	-2.77173400	-0.71629900
H	-7.27482500	1.10342300	0.42543700
H	-2.29724900	-0.93694100	0.38373700
H	-2.33724200	1.38964500	1.36623200
H	-4.73192100	2.18929600	1.30980300

35H (Charge = 1, Multiplicity = 1):

C	-7.13365600	-1.06417400	-0.75584500
C	-6.27963600	-2.14793900	-1.04688800
C	-4.92711000	-2.11559000	-0.74593900
C	-4.45939000	-0.95007600	-0.13856200
C	-5.30666000	0.12448400	0.15097400
C	-6.66792800	0.09325700	-0.15226200
N	-3.19246500	-0.57975400	0.29222300
C	-3.26950200	0.64260200	0.81069400
N	-4.51692000	1.09950700	0.74577300
C	-4.98697400	2.39804000	1.21571000
C	-1.99077800	-1.40042100	0.18991400
H	-8.18484000	-1.14024200	-1.01199100
H	-6.69481900	-3.03127000	-1.51983700
H	-4.26528200	-2.94535500	-0.96759700
H	-7.31927100	0.92995100	0.07456200
H	-2.43425500	1.18790500	1.22775500
H	-5.39763200	2.95558200	0.37304000
H	-5.75560200	2.24620600	1.97436500
H	-4.14276100	2.93595700	1.64361800
H	-1.15754800	-0.84619300	0.61839800
H	-2.14540000	-2.32863600	0.74137500
H	-1.79506800	-1.61716900	-0.86094400

36H (Charge = 1, Multiplicity = 1):

C	-4.82414600	-0.03563400	0.59156800
C	-4.69191300	0.09399400	-0.83430700
C	-3.44307900	-0.09952100	-1.46402400

C	-2.37872300	-0.41337900	-0.65503700
C	-2.50888400	-0.54136100	0.74991800
C	-3.70815300	-0.35932700	1.39397700
N	-1.03697200	-0.66534500	-0.93313900
C	-0.39368100	-0.92631500	0.19603700
N	-1.23610900	-0.86229500	1.21741600
C	-6.10764300	0.16852000	1.18192400
C	-7.19208700	0.48114900	0.41110700
C	-7.06110100	0.60969700	-1.00012600
C	-5.84913800	0.42189400	-1.60319800
H	-3.33836600	-0.00201300	-2.53923900
H	-3.80387200	-0.45865700	2.46984600
H	-0.60303400	-0.65664200	-1.85142800
H	0.65871600	-1.15736400	0.27234000
H	-0.97562600	-1.02003300	2.18625500
H	-6.19993200	0.06830600	2.25953100
H	-8.16216200	0.63326500	0.87328100
H	-7.93307700	0.85826100	-1.59647100
H	-5.74104700	0.51804200	-2.67970400

37H (Charge = 1, Multiplicity = 1):

C	-2.41076900	0.26755500	-1.58558200
C	-2.38654200	1.50427900	-0.91416200
C	-3.20542400	1.75554000	0.17441300
C	-4.06012400	0.72882900	0.58135400
C	-4.07903700	-0.49872300	-0.08923600
C	-3.25419200	-0.75320400	-1.18650900
S	-5.21071600	0.71506500	1.89866900
C	-5.65489900	-0.87790400	1.51416000
N	-5.00221200	-1.36336500	0.48831100
H	-1.75377900	0.11158000	-2.43396300
H	-1.71101100	2.28041600	-1.25668600
H	-3.18518700	2.70834700	0.69092800
H	-3.28600900	-1.71176300	-1.69192300
H	-6.40269900	-1.44623400	2.05463000
H	-5.16457800	-2.31156000	0.14553400

38H (Charge = 1, Multiplicity = 1):

C	-2.47045900	0.38845500	-1.78043200
C	-2.34549300	1.70107800	-1.29212000
C	-3.06016600	2.13293500	-0.18633000
C	-3.91117300	1.21142400	0.42573200
C	-4.03268000	-0.09292000	-0.06256600
C	-3.31316000	-0.52898600	-1.17703400
S	-4.94068900	1.43141200	1.82081400
C	-5.46943000	-0.18053400	1.69168900
N	-4.93482700	-0.84386300	0.69734700
C	-5.24164400	-2.24496700	0.38652600
H	-1.89488800	0.08740100	-2.64868600
H	-1.67490200	2.39211400	-1.79103800
H	-2.96458300	3.14515200	0.18988800
H	-3.41346100	-1.54284000	-1.54782300
H	-6.18741700	-0.63009000	2.36858900

H	-5.65601200	-2.29109400	-0.62100600
H	-4.31723500	-2.82054700	0.44283600
H	-5.96355100	-2.61107900	1.11302200

39H (Charge = 1, Multiplicity = 1):

C	-1.98364900	-0.39062900	0.31207500
C	-2.55012600	-1.67918100	0.27880600
C	-3.87846800	-1.89527800	-0.06809900
C	-4.59052200	-0.74886300	-0.37505600
C	-4.04415000	0.52698900	-0.34632500
C	-2.71518000	0.74706700	0.00027200
O	-5.91505700	-0.63859900	-0.75301700
C	-6.15570800	0.63651300	-0.94279400
N	-5.09658500	1.36714400	-0.71864800
H	-0.94118300	-0.28447800	0.59084600
H	-1.92986400	-2.53161900	0.53251100
H	-4.32881600	-2.87981300	-0.09820800
H	-2.28815800	1.74220800	0.02315500
H	-7.13557500	0.97944300	-1.24769600
H	-5.06703200	2.38185800	-0.81355400

40H (Charge = 1, Multiplicity = 1):

C	-1.97628400	-0.85877200	0.53040200
C	-2.54233000	-2.14644800	0.47899900
C	-3.85561400	-2.36350200	0.07698800
C	-4.55382600	-1.21872700	-0.26500900
C	-4.00726900	0.05534900	-0.21856200
C	-2.69446200	0.27791600	0.18232700
O	-5.85957000	-1.10598400	-0.69609600
C	-6.08210200	0.17479600	-0.89746900
N	-5.03541000	0.91042300	-0.63553100
C	-4.94475300	2.36561900	-0.75436200
H	-0.94647500	-0.75201300	0.85255000
H	-1.93438800	-2.99843500	0.76249300
H	-4.30436300	-3.34830300	0.03340900
H	-2.26711500	1.27318600	0.21890700
H	-7.04694900	0.52233000	-1.24344800
H	-4.70439900	2.77560100	0.22645700
H	-4.15842700	2.60307400	-1.47052100
H	-5.90578200	2.74061000	-1.10095900

41H (Charge = 1, Multiplicity = 1):

C	-5.29601800	-2.28924800	0.24001600
C	-6.69223700	-2.11060700	0.09264200
C	-7.24703800	-0.85981100	-0.02163400
C	-6.42680200	0.30141500	0.00622300
C	-5.02993000	0.12885400	0.15318800
C	-4.49272500	-1.17926400	0.26700300
C	-6.93083700	1.62640000	-0.10475100
C	-6.07989000	2.70343900	-0.06902200
C	-4.68205400	2.53680400	0.07756200
C	-4.18171600	1.26556200	0.18501600
N	-2.80143100	1.00858400	0.33355500

C	-2.31088400	-0.20735900	0.43784100
N	-3.09061600	-1.26614500	0.40844500
H	-4.86389800	-3.28040000	0.32922100
H	-7.32886200	-2.98877000	0.07061900
H	-8.31965000	-0.73793800	-0.13490900
H	-8.00078200	1.76974600	-0.21822400
H	-6.47695700	3.70936700	-0.15456600
H	-4.01557900	3.39250100	0.10417500
H	-1.24206100	-0.33971800	0.55098000
H	-2.15405400	1.79195000	0.36440400
H	-2.65913300	-2.18307500	0.49088700

42H (Charge = 1, Multiplicity = 1):

C	-5.29361900	-2.28831800	0.23418300
C	-6.68722900	-2.10719900	0.07380700
C	-7.23743300	-0.85643000	-0.03992300
C	-6.41276100	0.29961100	0.00162000
C	-5.01462200	0.12914500	0.16168900
C	-4.47959500	-1.18166300	0.27565100
C	-6.92713000	1.61904900	-0.11012600
C	-6.08434600	2.69959200	-0.06344200
C	-4.68778500	2.54032900	0.09514400
C	-4.17109300	1.27130100	0.20454900
N	-2.78399100	1.02965500	0.36397400
C	-2.31988100	-0.20063200	0.46596700
N	-3.07528500	-1.28100000	0.43110200
C	-2.45946800	-2.60519700	0.54953000
C	-1.86054500	2.16646000	0.41506000
H	-4.88820300	-3.28829800	0.32107700
H	-7.32308900	-2.98559700	0.04172300
H	-8.30820100	-0.72830800	-0.16330200
H	-7.99728900	1.75265800	-0.23305300
H	-6.48410800	3.70440100	-0.14950100
H	-4.04872300	3.41359000	0.12655700
H	-1.25052700	-0.33399100	0.58428000
H	-2.87117300	-3.11505600	1.42216600
H	-2.67207100	-3.18083400	-0.35301600
H	-1.38473000	-2.48303500	0.66635700
H	-0.84540400	1.79315900	0.53656000
H	-1.93791800	2.73213300	-0.51500900
H	-2.12389700	2.80344800	1.26123900

43H (Charge = 1, Multiplicity = 1):

C	-4.93064300	-0.57087200	0.28116400
C	-3.77345900	-1.06584300	-0.34992000
N	-3.66327400	-2.39421500	-0.48045600
C	-4.57460700	-3.36340800	-0.05680400
N	-5.68597700	-2.80112000	0.56039400
C	-5.86321100	-1.49316100	0.72122100
C	-2.65311100	-0.24988200	-0.89097200
O	-4.40977400	-4.54472400	-0.21247900
C	-5.26859900	0.85994500	0.53193300
O	-6.30717500	1.19096200	1.05804700

O	-4.32762800	1.69945900	0.12648900
C	-3.38816000	3.86620900	-0.15109400
C	-4.59327500	3.10606200	0.34631400
H	-2.83336400	-2.77205900	-0.93937500
H	-6.39303500	-3.45335800	0.89843600
H	-6.77521900	-1.17903200	1.21826600
H	-3.04023500	0.45134500	-1.63331500
H	-2.21530100	0.34154700	-0.08346200
H	-1.89296600	-0.88909200	-1.34000300
H	-3.55158400	4.93635000	-0.00336200
H	-2.49084800	3.57317900	0.39977800
H	-3.22606400	3.68371700	-1.21636300
H	-5.50421600	3.37096800	-0.19649100
H	-4.76783800	3.25899900	1.41419400

44H (Charge = 1, Multiplicity = 1):

C	-2.72333400	-0.34778800	-0.23664700
C	-3.20938500	0.92034000	0.08250100
N	-4.55438000	1.04992700	0.09012600
C	-5.40210800	0.02980500	-0.18832900
N	-4.97659700	-1.17834400	-0.49604900
C	-3.65760300	-1.34978200	-0.51702800
C	-2.42369300	2.14083900	0.41557000
C	-1.28323600	-0.74200600	-0.30541100
O	-0.93790100	-1.86952000	-0.57477400
O	-0.45500200	0.25858900	-0.04383400
C	1.70485000	1.20881100	0.25164600
C	0.95756000	-0.05674500	-0.09114600
O	-6.66150400	0.34988500	-0.12372100
C	-7.63043300	-0.68485000	-0.41773300
H	-4.96328500	1.95949700	0.31353900
H	-3.29789800	-2.34342000	-0.76928800
H	-1.79594000	1.94362700	1.28713900
H	-1.76104900	2.38775500	-0.41645800
H	-3.08918900	2.97956400	0.62135800
H	2.77902400	1.01072100	0.22675300
H	1.48104500	1.99925400	-0.46910600
H	1.43956800	1.55632900	1.25329600
H	1.15339800	-0.86007000	0.62342800
H	1.19368400	-0.41929000	-1.09485200
H	-8.59550100	-0.19764000	-0.30518200
H	-7.48831500	-1.04030800	-1.43838800
H	-7.52054600	-1.50350600	0.29348100

45H (Charge = 1, Multiplicity = 1):

C	-4.82219600	-0.51616500	0.49342900
C	-3.69130800	-1.04330800	-0.15635800
N	-3.60489900	-2.37939600	-0.25437400
C	-4.50837300	-3.31432000	0.20977200
N	-5.58687000	-2.73102700	0.83300700
C	-5.75176700	-1.41777800	0.97770700
S	-4.31311900	-4.93797400	0.03348000
C	-2.57496200	-0.26128100	-0.74965000

C	-5.13272900	0.92645300	0.72238100
O	-6.11909500	1.27746400	1.32832800
O	-4.23420700	1.74268200	0.19637100
C	-3.37007600	3.89249700	-0.33977200
C	-4.47831500	3.15995500	0.37587600
H	-2.78642900	-2.76804000	-0.72508900
H	-6.29922100	-3.36104700	1.20171600
H	-6.64856900	-1.09146000	1.49429400
H	-2.97092800	0.39938400	-1.52460500
H	-2.12744000	0.37164900	0.01988200
H	-1.82152100	-0.92507000	-1.17324700
H	-3.51911500	4.96886000	-0.22621300
H	-2.39592000	3.63087600	0.08077400
H	-3.37282000	3.65257000	-1.40597900
H	-5.46287300	3.39219300	-0.03720500
H	-4.49122200	3.37065700	1.44828400

46H (Charge = 1, Multiplicity = 1):

C	-5.68791100	-3.52538900	0.64768600
C	-5.98340400	-3.14235900	1.97957800
C	-6.19353200	-1.82513100	2.32932000
C	-6.10612100	-0.85988100	1.32339000
C	-5.81314600	-1.20764800	-0.01978000
C	-5.60393600	-2.57831900	-0.33781100
O	-6.31007000	0.42033300	1.67240300
C	-6.24956800	1.41608800	0.77376500
C	-5.96249900	1.14729900	-0.58880000
C	-5.74529100	-0.18134300	-0.96696200
C	-6.47973500	2.71511800	1.23314800
C	-6.42138200	3.74353500	0.31630200
C	-6.13802100	3.51116600	-1.05250700
C	-5.91165700	2.23747900	-1.50144600
H	-5.53010200	-4.57266200	0.41756200
H	-6.04695300	-3.90668800	2.74724100
H	-6.42019100	-1.52390900	3.34534000
H	-5.37972600	-2.84027800	-1.36669400
H	-5.52291200	-0.41782000	-2.00520400
H	-6.69517400	2.88437000	2.28175900
H	-6.59740000	4.75963500	0.65379800
H	-6.10261700	4.34949900	-1.73858600
H	-5.69191500	2.02807700	-2.54327000

47H (Charge = 1, Multiplicity = 1):

C	-7.39764000	0.03477500	0.69964700
C	-7.34191400	1.41674700	0.40904800
C	-6.14198000	2.05782200	0.18388300
C	-4.94699500	1.32160100	0.24495800
C	-4.97811200	-0.07196800	0.53689700
C	-6.24069500	-0.69445000	0.76170800
S	-3.48161700	2.18089700	-0.04819200
C	-2.23755200	0.99811000	0.10648200
C	-2.50521500	-0.36594700	0.41511700
C	-3.80894800	-0.84020100	0.60977800

C	-0.91563700	1.43292300	-0.08617300
C	0.11662500	0.52588500	0.02884500
C	-0.12451700	-0.83227800	0.33644200
C	-1.40804300	-1.26931000	0.52514900
H	-8.35657200	-0.44019900	0.87220900
H	-8.26204000	1.98978900	0.36137600
H	-6.11824300	3.11988000	-0.03810000
H	-6.25333700	-1.75658100	0.98449000
H	-3.92226900	-1.89848500	0.83780200
H	-0.71179000	2.47237300	-0.32221500
H	1.13603300	0.86637000	-0.12043200
H	0.70854400	-1.52062300	0.42058900
H	-1.62394600	-2.30631600	0.76205900

Electron spin density of transition states











