Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

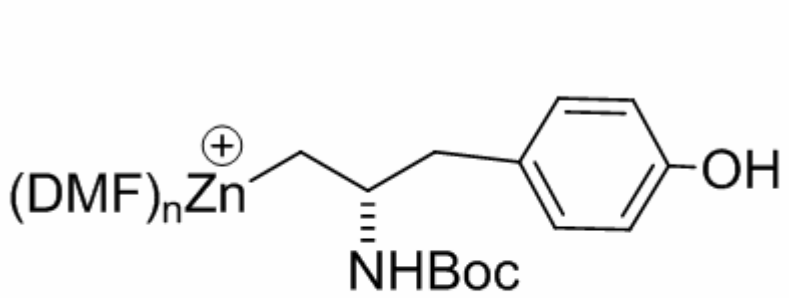
Gas-phase study of new organo-zinc reagents by IRMPD-Spectroscopy, Computational modeling and Tandem-MS:

Supplementary Information:
Figures 1S - 3S
Schemes 1S - 7S

Ahmad R. Massah,[1] Frank Dreiocker,[2] Richard F.W. Jackson,[1]
Barry T. Pickup,[1] Jos Oomens,[3,4] Anthony J. H. M. Meijer,[1] and Mathias Schäfer[2]

[1]Department of Chemistry, The University of Sheffield, Sheffield, S3 7HF, United Kingdom
[2]Department of Chemistry, University of Cologne, Greinstrasse 4, 50939 Köln, Germany
[3]FOM Institute for Plasma Physics Rijnhuizen, Edisonbaan 14, Nieuwegein 3439 MN, The Netherlands
[4]University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands
(Dated: March 9th, 2011)

Scheme 1S.
Combined ESI-MS/MS fragmentation pattern of precursor ions **1a** and **1b**, respectively. ESI-MS/MS of **1a** delivers exclusively product ion **1b** upon loss of DMF. Successive MS/MS of ion **1b** yields the depicted product ions. The structures of the product ions are consistent with exact ion masses determined.



1a, n = 2
1b, n = 1

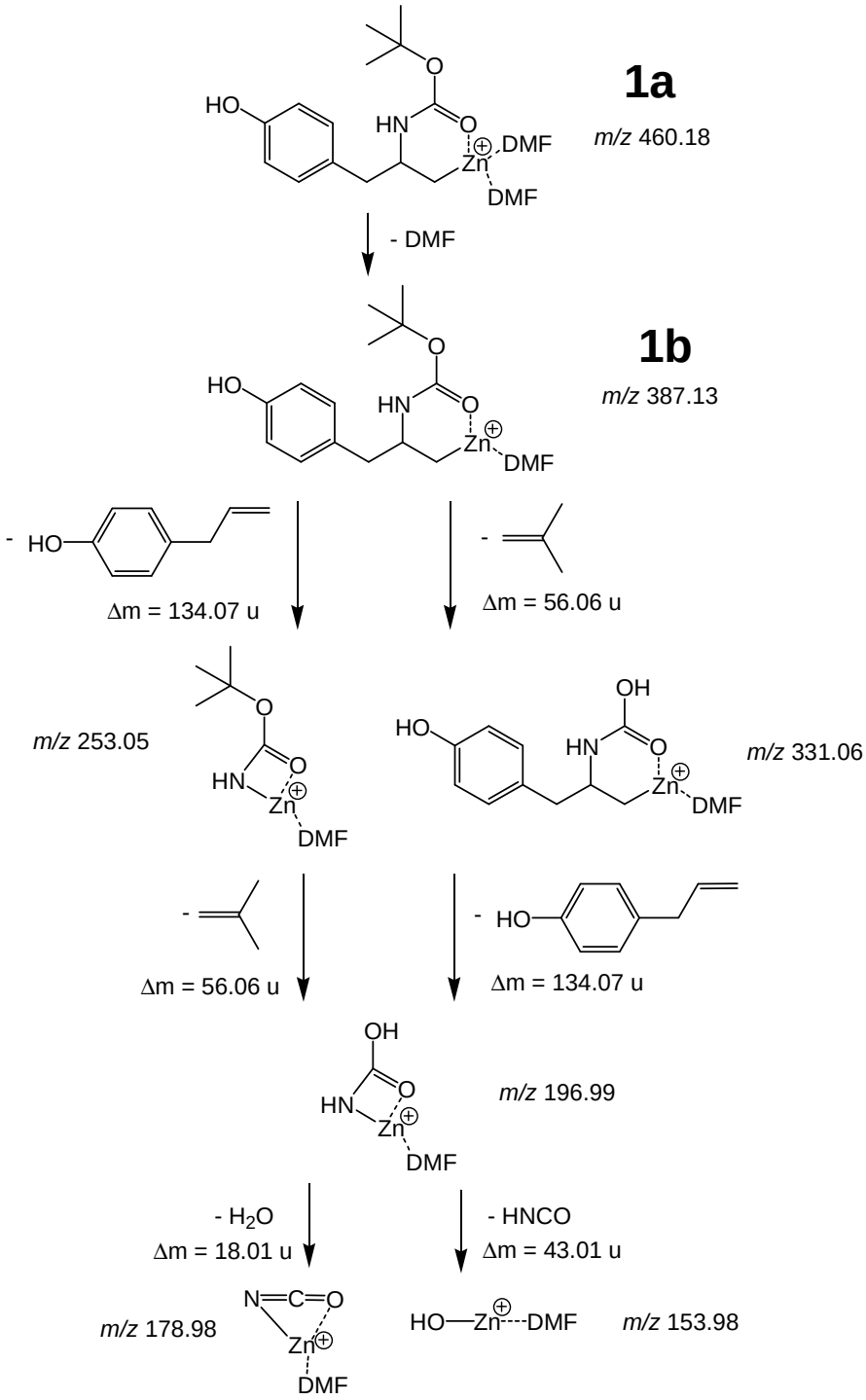
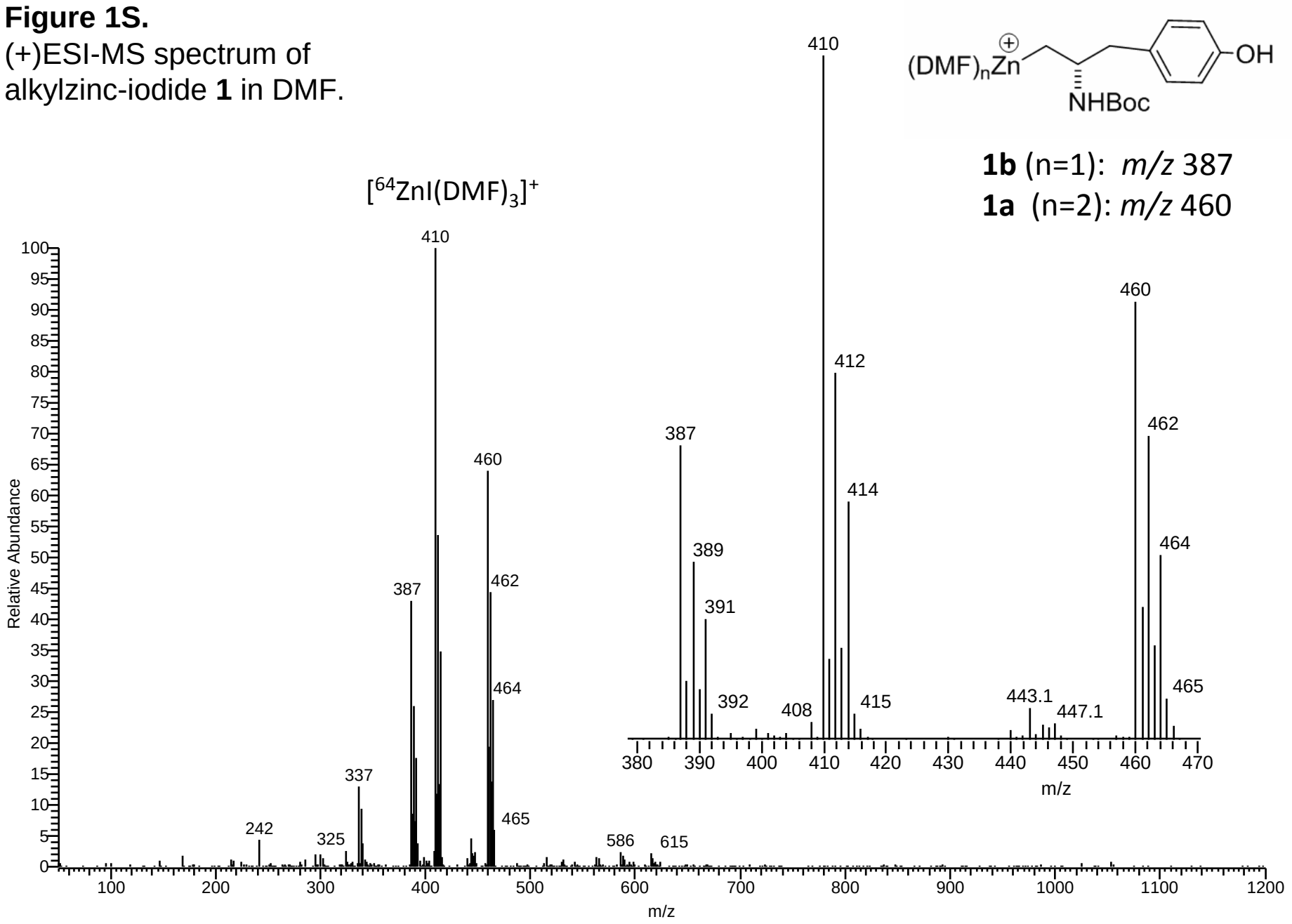
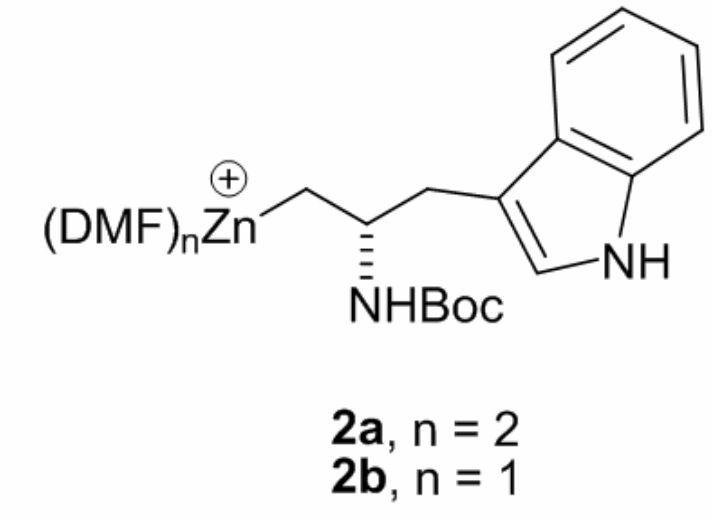
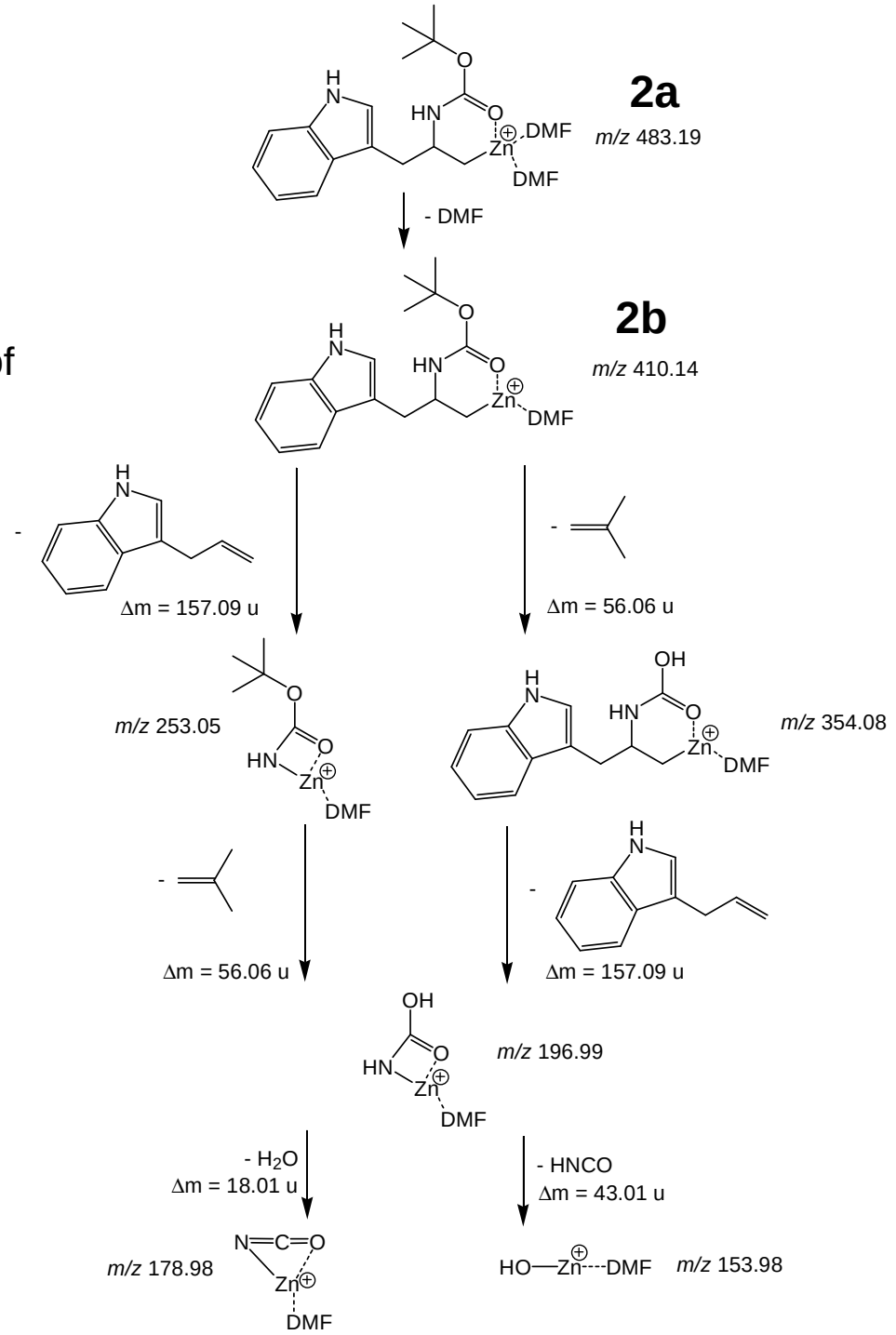


Figure 1S.
(+)ESI-MS spectrum of alkylzinc-iodide **1** in DMF.

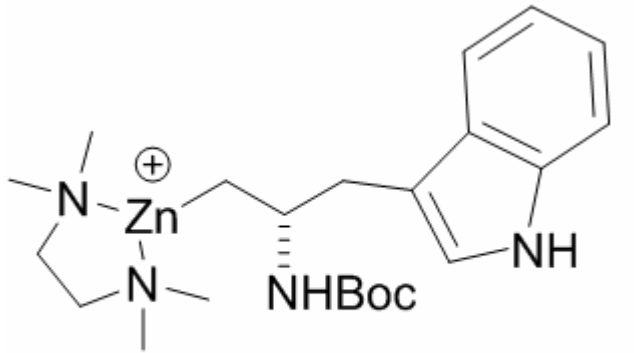


Scheme 2S.
Combined ESI-MS/MS fragmentation pattern of precursor ions **2a** and **2b**, respectively. ESI-MS/MS of **2a** delivers exclusively product ion **2b** upon loss of DMF. Successive MS/MS of ion **2b** yields the depicted product ions. The structures of the product ions are consistent with exact ion masses determined.

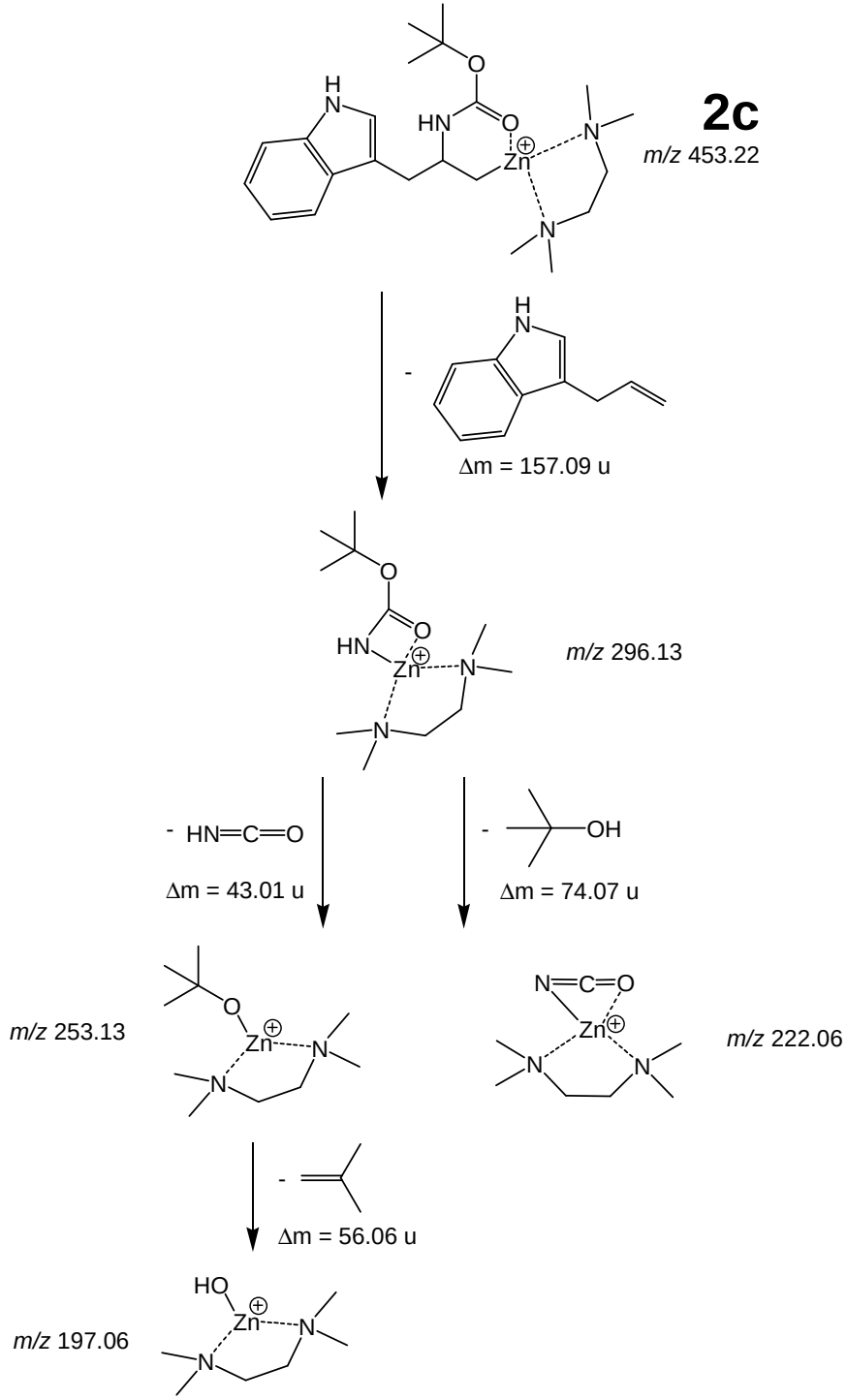




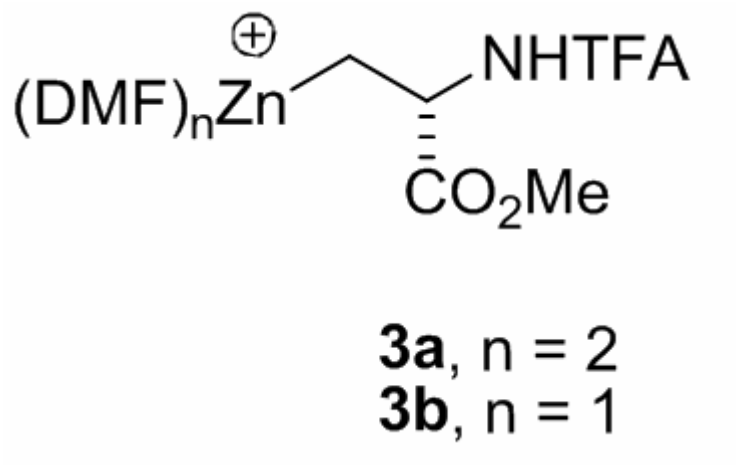
Scheme 3S.
ESI-MS/MS fragmentation pattern of precursor ion **2c**. The structures of the product ions are consistent with exact ion masses determined.

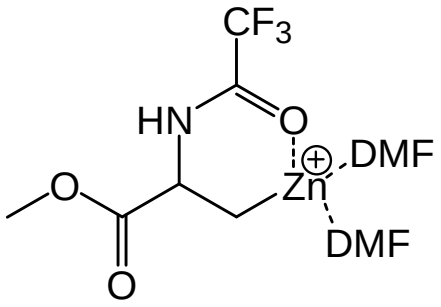


2c



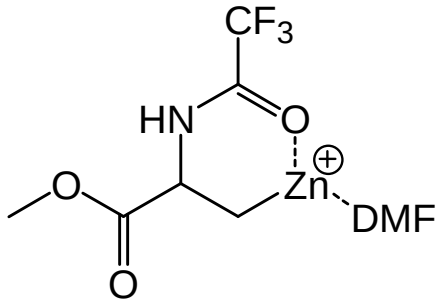
Scheme 4S.
Combined ESI-MS/MS fragmentation pattern of precursor ions **3a** and **3b**, respectively. ESI-MS/MS of **3a** delivers exclusively product ion **3b** upon loss of DMF. Successive MS/MS of ion **3b** yields the depicted product ion.



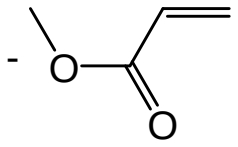


3a
m/z 408.07

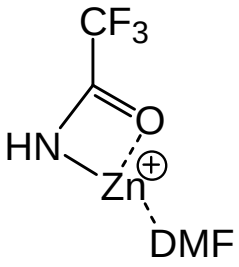
- DMF



3b
m/z 335.02

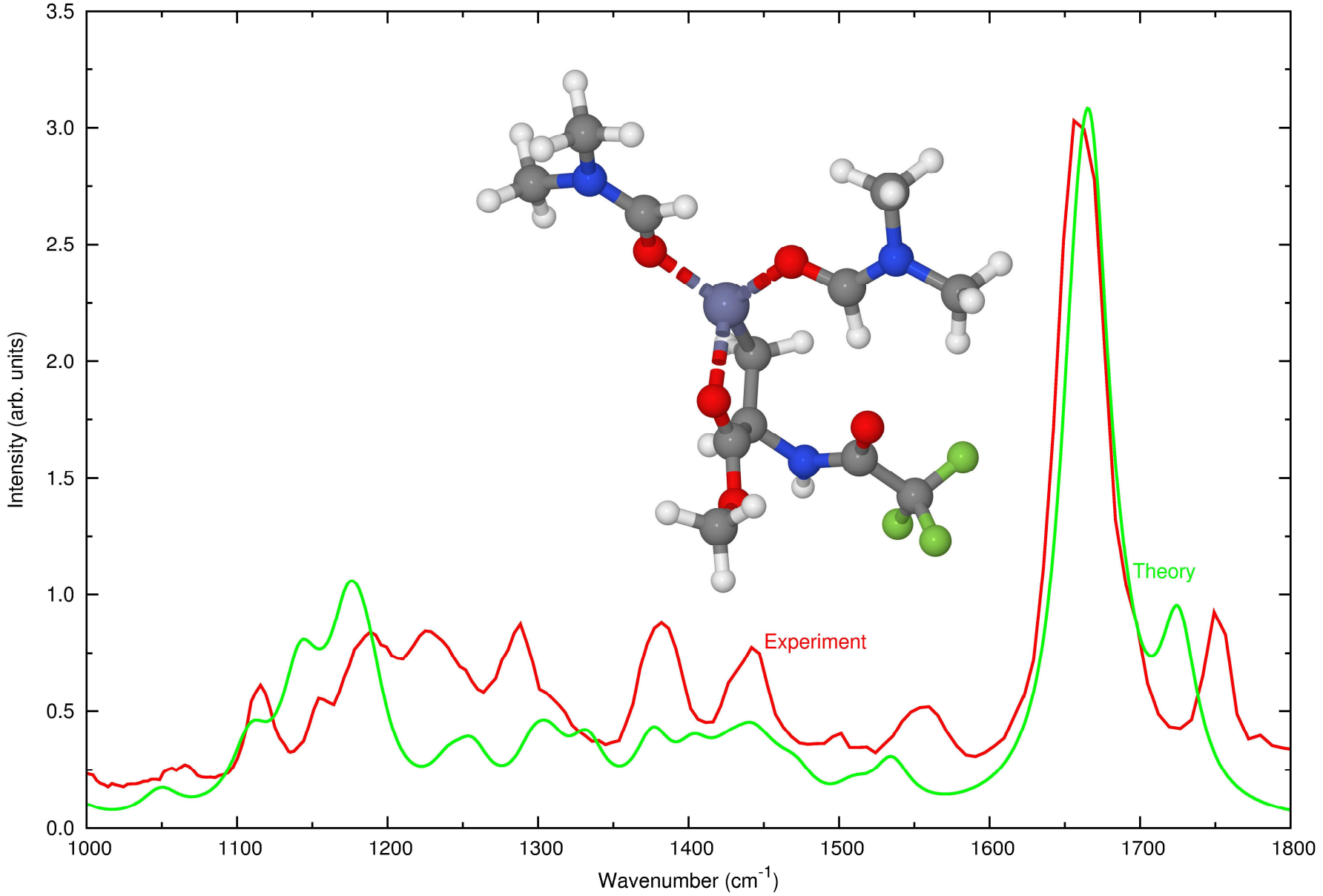


Δm = 86.04 u

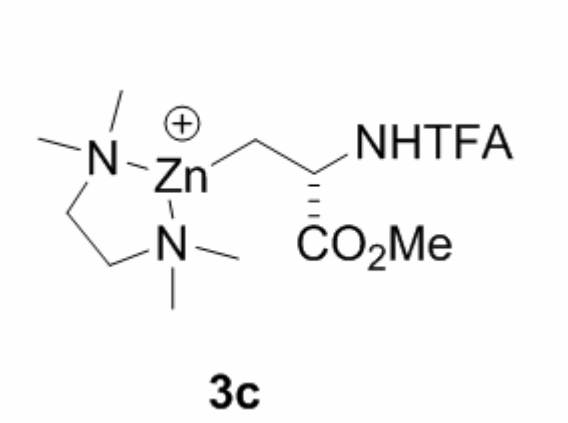


m/z 248.98

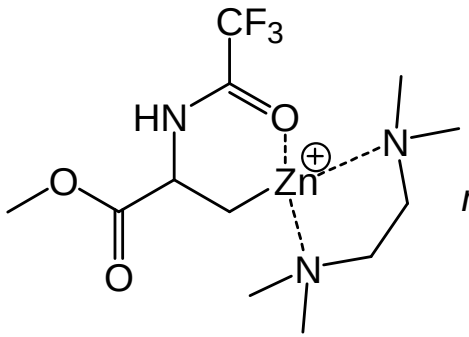
Figure 2S. IRMPD-spectrum of bis-DMF-organozinc-complex ion **3a** compared to the computed IR-spectrum of the conformer at +9.5 kJmol^{-1}.



Scheme 5S.
ESI-MS/MS fragmentation pattern of precursor ion **3c**. The structures of the product ions are consistent with exact ion masses determined.

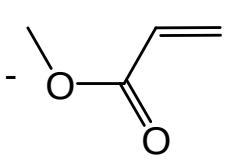


3c

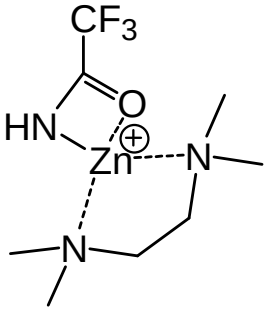


3c

m/z 378.10



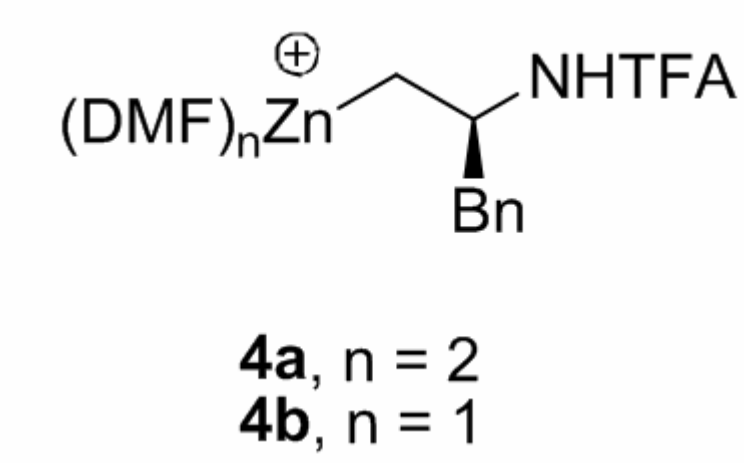
Δm = 86.04 u

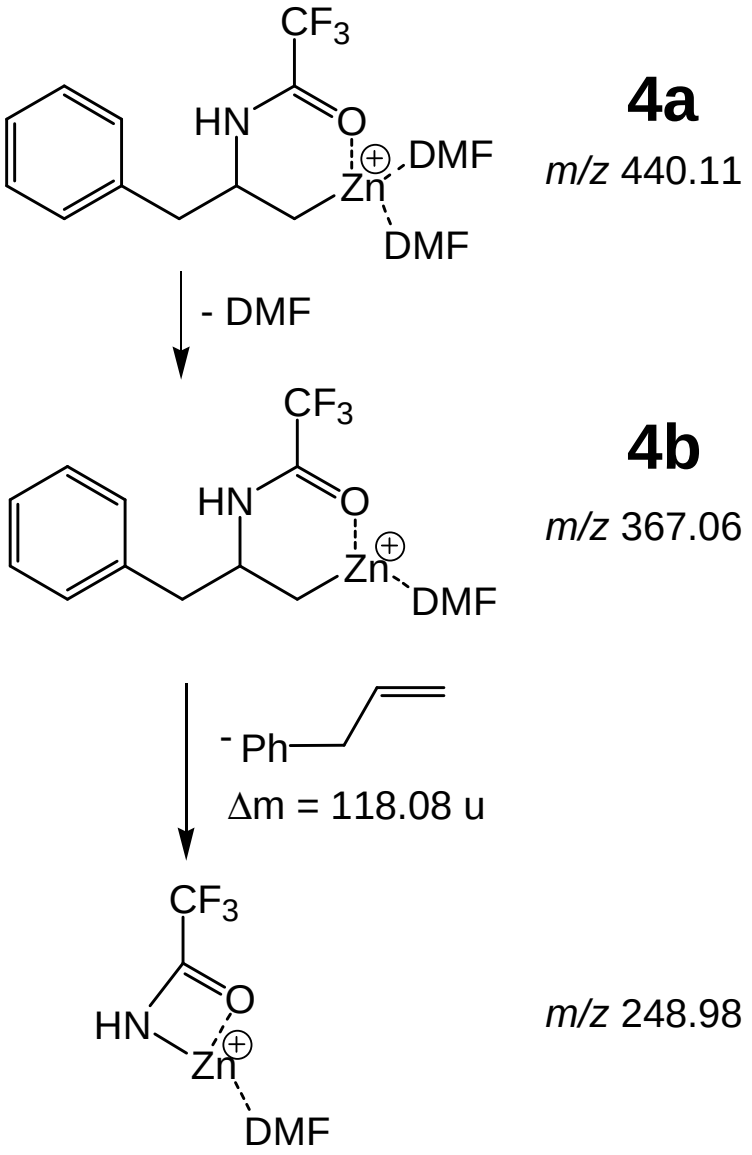


m/z 292.06

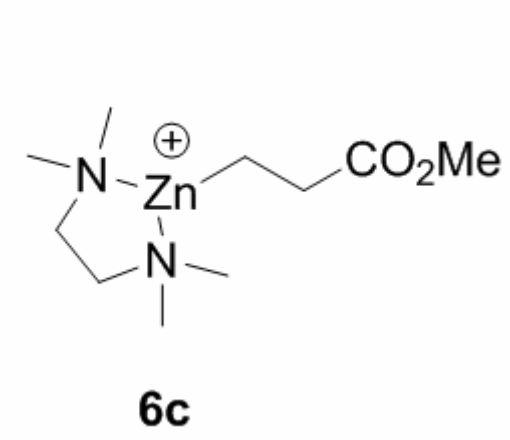
Scheme 6S.

Combined ESI-MS/MS fragmentation pattern of precursor ions **4a** and **4b**, respectively. ESI-MS/MS of **4a** delivers exclusively product ion **4b** upon loss of DMF. Successive MS/MS of ion **4b** yields the depicted product ion.





Scheme 7S.
ESI-MS/MS fragmentation pattern of precursor ion **6c**. The structures of the product ions are consistent with exact ion masses determined.



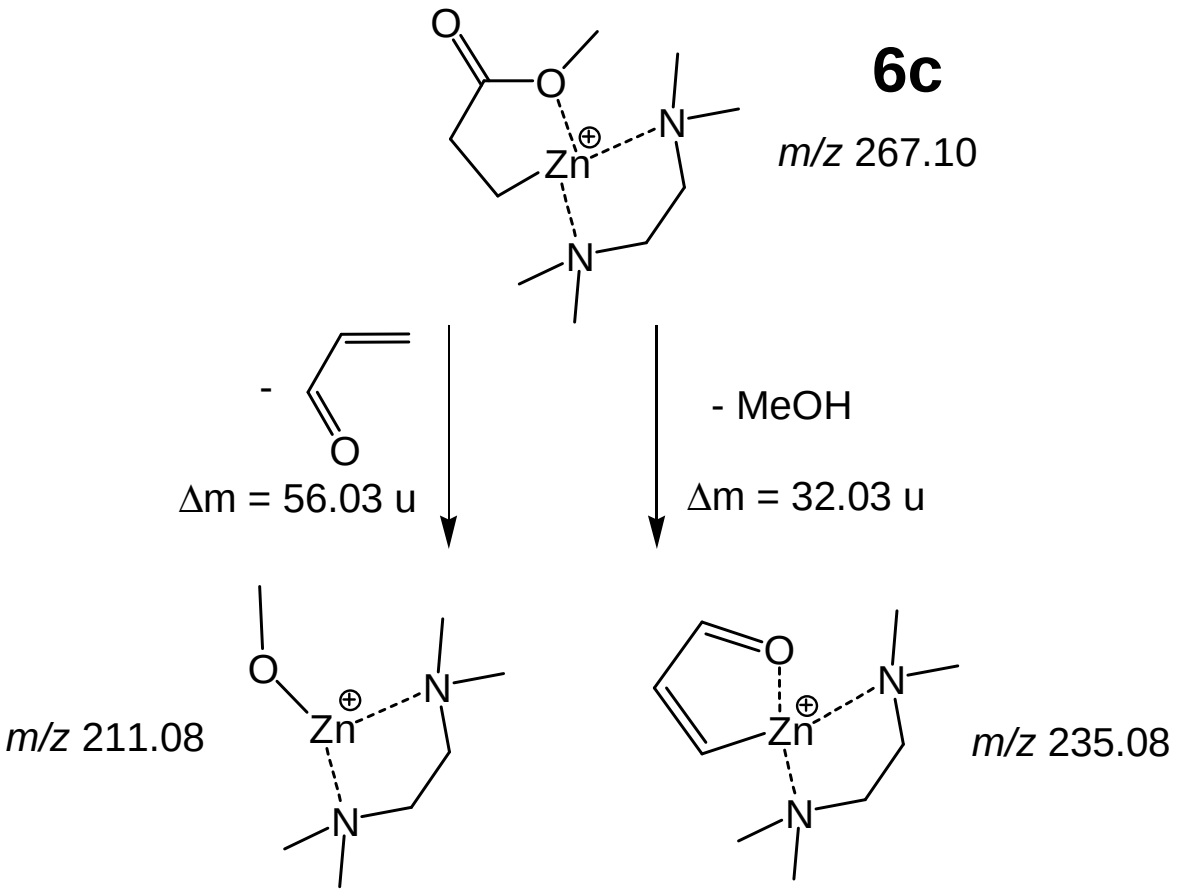
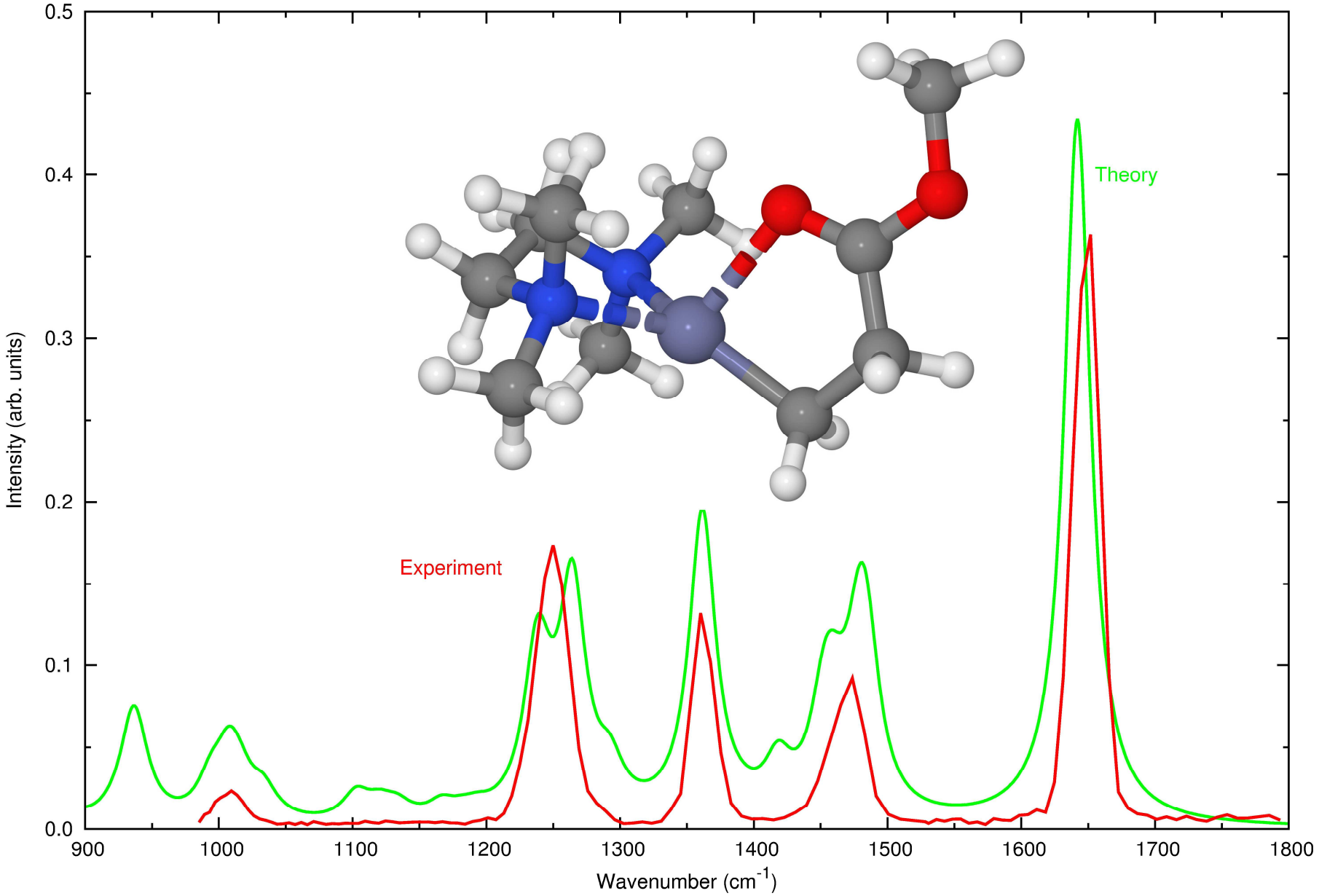


Figure 3S. IRMPD-spectrum of TMEDA-organozinc-complex ion **5c** compared to the computed IR-spectrum of the global minimum structure predicted by theory.



Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Gas-phase study of new organo-zinc reagents by IRMPD-Spectroscopy, Computational modeling and Tandem-MS:

Supplementary Information: Synthesis and analytic data set of the compounds analyzed in the gas phase

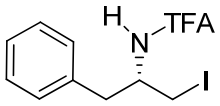
Ahmad R. Massah,[1] Frank Dreiocker,[2] Richard F.W. Jackson,[1]
Barry T. Pickup,[1] Jos Oomens,[3,4] Anthony J. H. M. Meijer,[1] and Mathias Schäfer[2]

[1]*Department of Chemistry, The University of Sheffield, Sheffield, S3 7HF, United Kingdom*
[2]*Department of Chemistry, University of Cologne, Greinstrasse 4, 50939 Köln, Germany*
[3]*FOM Institute for Plasma Physics Rijnhuizen, Edisonbaan 14, Nieuwegein 3439 MN, The Netherlands*
[4]*University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*
(Dated: February 25, 2011)

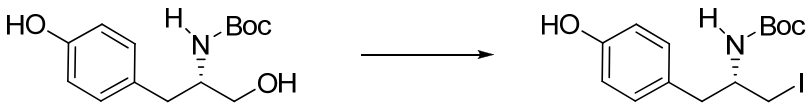
Materials

General procedure for Iodination

The alcohol (10.0 mmol) was added by syringe over 30 min to a stirred solution of triphenylphosphine (2.75 g, 10.5 mmol), imidazole (0.71 g, 10.5 mmol) and iodine (2.66 g, 10.5 mmol) in dry CH_2Cl_2 (30 mL) under nitrogen at 0 ^oC and the reaction mixture was left overnight at room temperature. The precipitate was removed by filtration, the filtrate was concentrated under reduced pressure and the residue dissolved in EtOAc (150 mL). The insoluble material was removed by filtration and the filtrate was washed with saturated aqueous sodium thiosulfate solution (50 mL) and brine (50 mL), dried over $MgSO_4$ and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography.



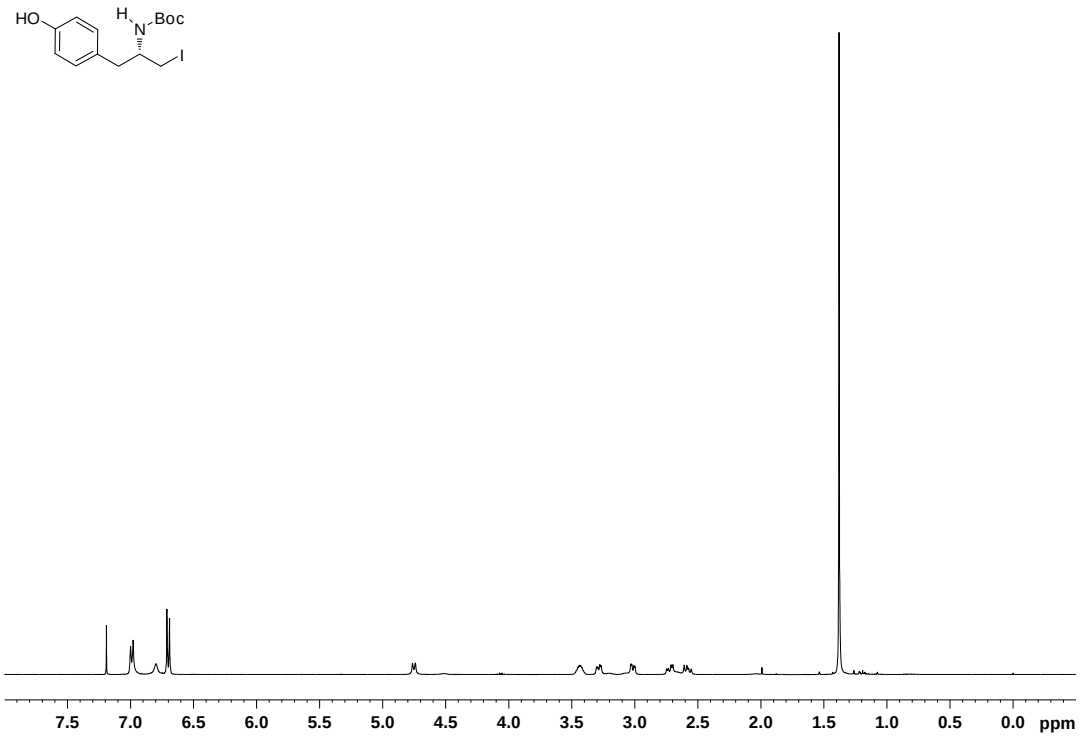
(S)-(+)-2,2,2-Trifluoro-N-(1-iodo-3-phenylpropan-2-yl)acetamide was prepared by the literature method.[1]



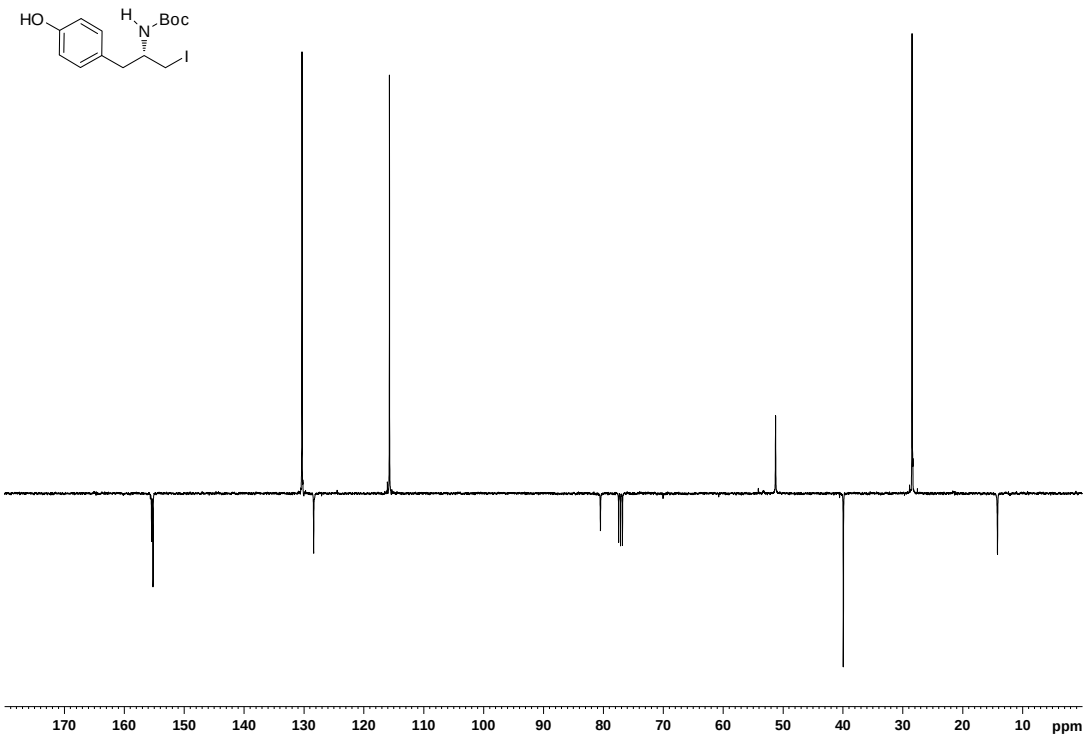
(S)-*tert*-Butyl 1-(4-hydroxyphenyl)-3-iodopropan-2-ylcarbamate

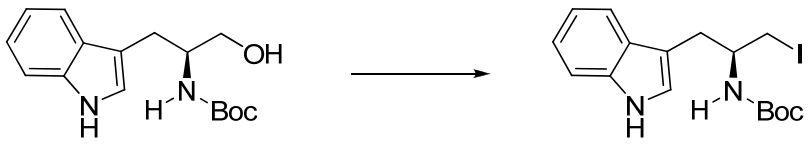
Treatment of the corresponding alcohol[2] using the standard iodination method, followed by column chromatography of the crude product (eluting with 10% EtOAc:90% 40-60 petrol to 30% EtOAc:70% 40-60 petrol) gave the title compound (15 %) as a white solid, mp 126-128 ^{o}C; R_f 0.18 (20 % EtOAc in petrol); FTIR (ν_{max}/ cm^{-1}): 3314, 3175, 2965, 1667, 1597, 1546, 1514, 1450, 1335, 1297, 1231, 1159, 1009; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.38 (s, 9H), 2.58 (dd, *J* 14.0, 8.0 Hz, 1H), 2.72 (dd, *J* 14.0, 5.5 Hz, 1H), 3.02 (dd, *J* 10.5, 4.0 Hz, 1H), 3.28 (dd, *J* 10.5, 4.0 Hz, 1H), 3.39-3.48 (m, 1H), 4.72-4.78 (br, 1H), 6.70 (d, *J* 8.5, 2H), 6.80 (br, 1H), 6.99 (d, *J* 8.5, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 28.5, 40.0, 51.4, 80.6, 115.8, 128.6, 130.4, 155.2, 155.4, $[\alpha]_D^{22}$ +16.9 (c 1.0, $CHCl_3$); *m/z* (ES) Found: MNa^+ 400.0404. $C_{14}H_{20}INO_3Na$ requires MH^+ 400.0386.

^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (100 MHz, $CDCl_3$):

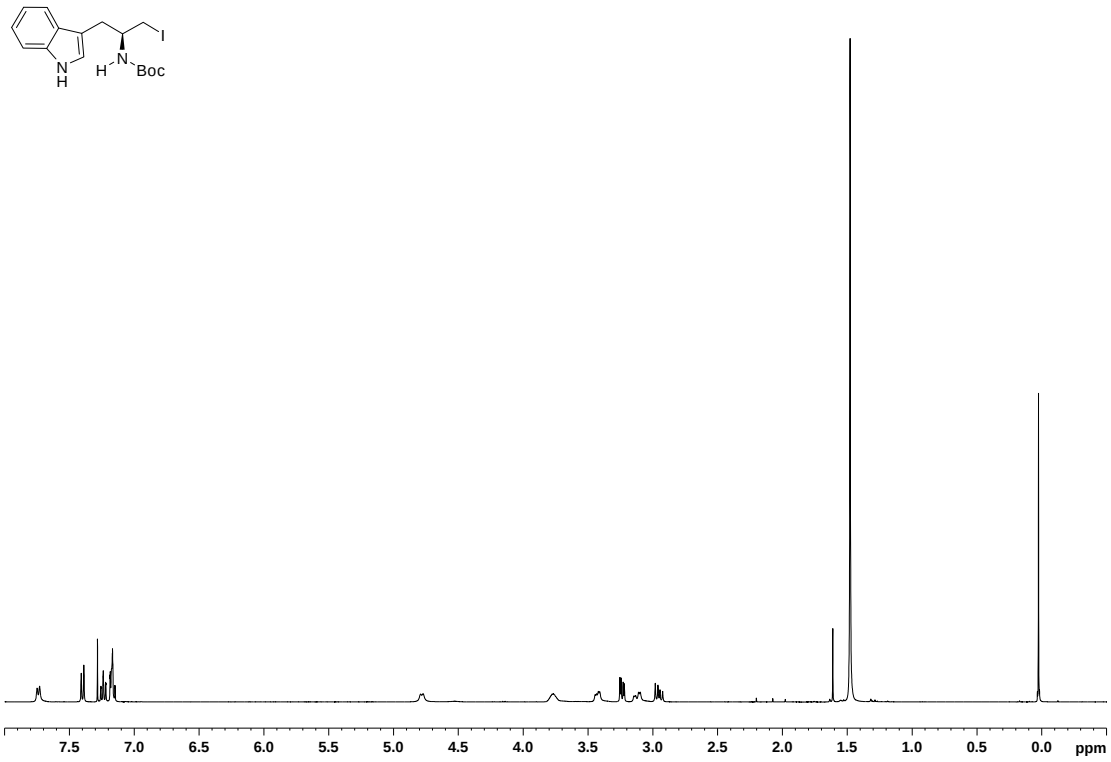




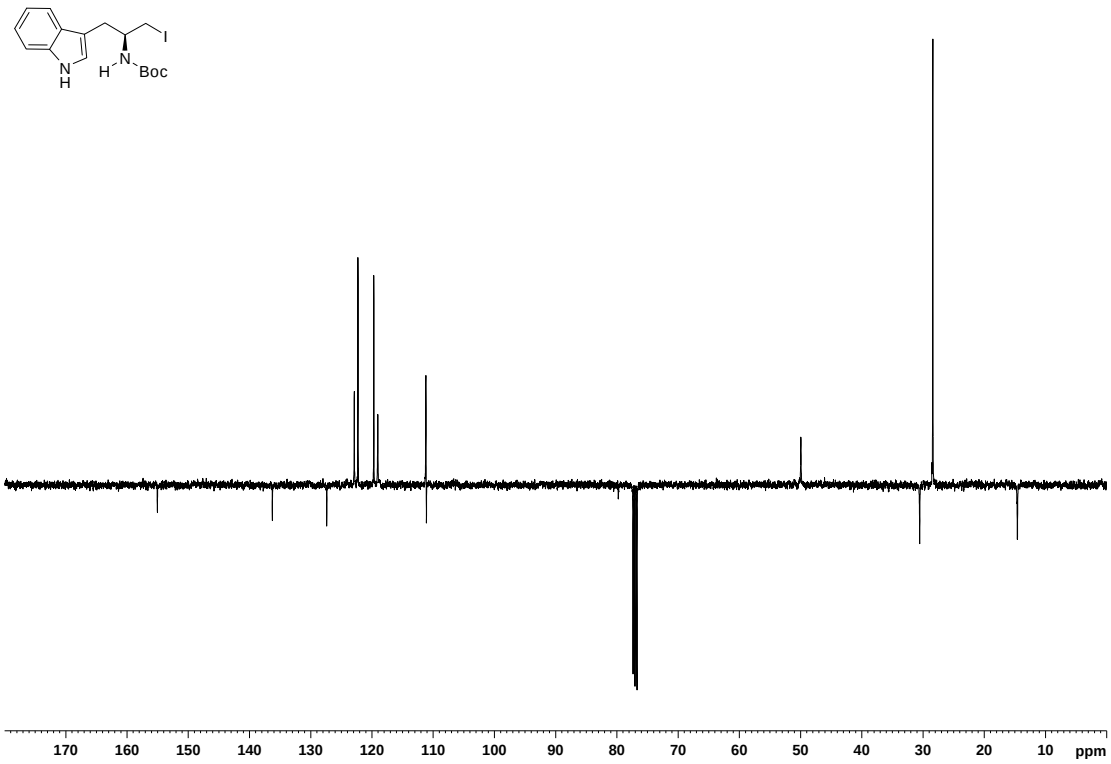
(S)-*tert*-Butyl 1-(1H-indol-3yl)-3-iodopropan-2-ylcarbamate

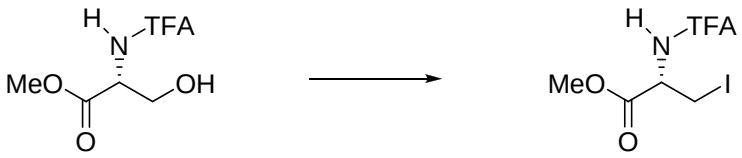
Treatment of the corresponding alcohol[3] using the standard iodination method, followed by column chromatography of the crude product (eluting with 5% EtOAc:95% 40-60 petrol to 10% EtOAc:90% 40-60 petrol) gave the title compound (65 %) as a white solid, mp 135.5-137 ^{o}C; R_f 0.25 (20 % EtOAc in petrol); FTIR (ν_{max}/ cm^{-1}): 3397, 3357, 2982, 1681, 1609, 1555, 1525, 1273, 1247, 1164, 1043; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.45 (s, 9H), 2.93 (dd, *J* 14.5, 8.5 Hz, 1H), 3.10 (dd, *J* 14.5, 5.0 Hz, 1H), 3.21 (dd, *J* 10.0, 4.0 Hz, 1H), 3.40 (dd, *J* 10.0, 4.0 Hz, 1H), 3.64-3.80 (m, 1H), 4.69-4.82 (br, 1H), 7.14 (m, 2H), 7.21 (dt, *J* 7.5, 1.0 Hz, 1H), 7.37 (d, *J* 8.0 Hz, 1H), 7.71 (d, *J* 8.0 Hz, 1H), 8.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.6, 28.5, 30.6, 50.0, 79.8, 111.1, 111.2, 119.1, 119.8, 122.3, 122.9, 127.4, 136.3, 155.1; $[\alpha]_D^{22}$ +27.2 (c 1.03, $CHCl_3$); *m/z* (ES) Found: MNa^+ 423.0532. $C_{16}H_{21}IN_2O_2Na$ requires MNa^+ 423.0545.

^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (100 MHz, $CDCl_3$):

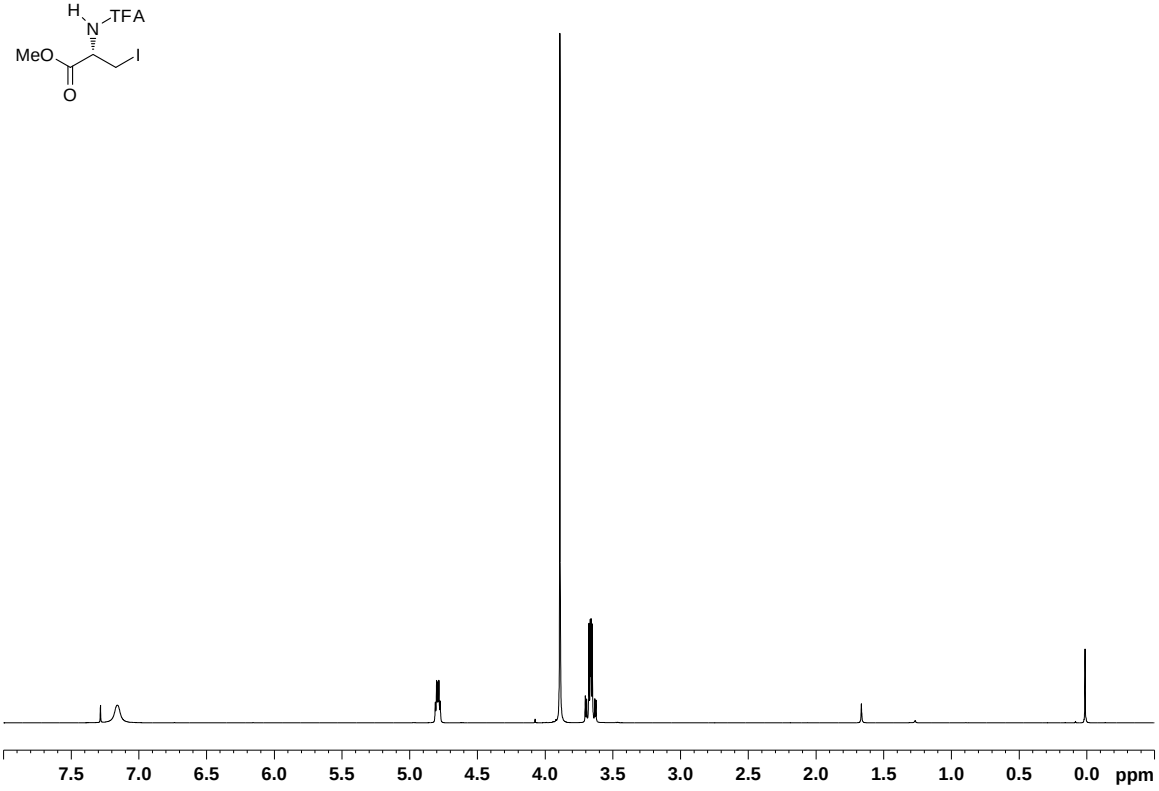




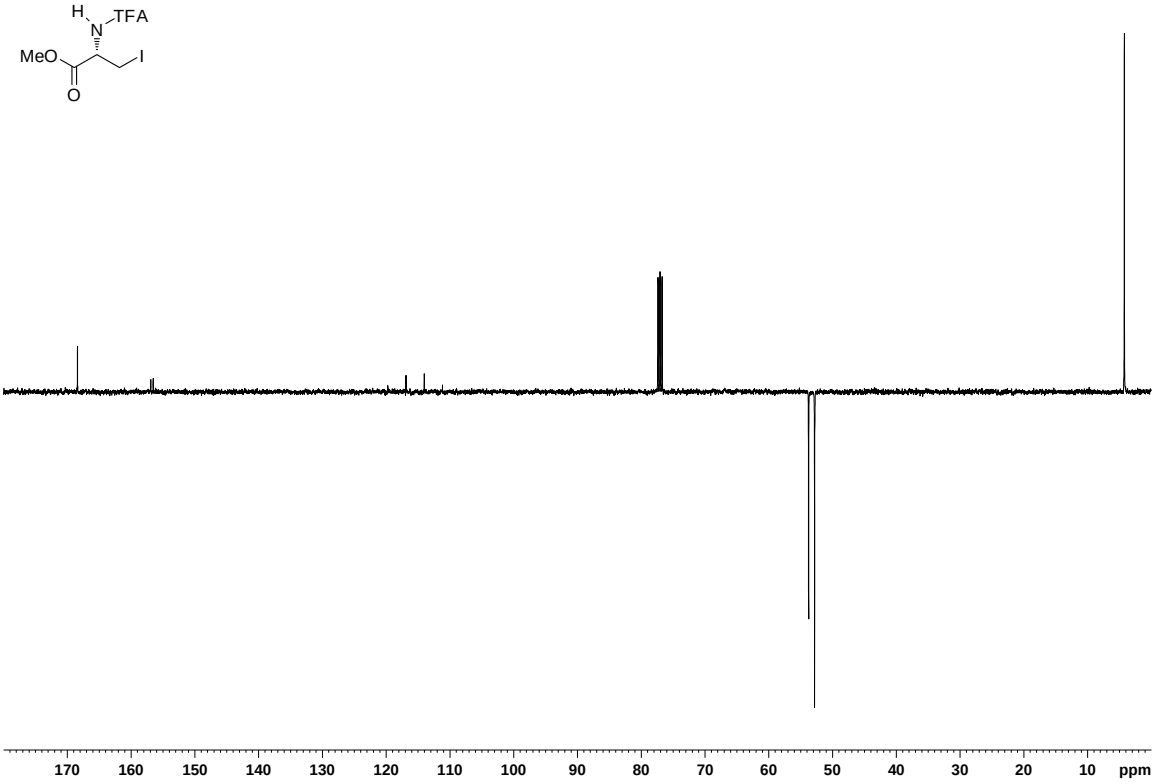
(S)-Methyl 3-iodo-2-(2,2,2-trifluoroacetamido)propanoate

Treatment of the corresponding alcohol[4] using the standard iodination method, followed by column chromatography of the crude product (eluting with 10% EtOAc: 90% 40-60 petrol to 15% EtOAc:85% 40-60 petrol) gave the title compound (25 %) as a white solid, mp 86-88 ^{o}C; R_f 0.31 (20 % EtOAc in petrol); FTIR (ν_{max}/ cm^{-1}) 3266, 3110, 2952, 1739, 1705, 1562, 1434, 1301, 1232, 1163, 1109, 1011, 924; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (dd, *J* 11.0, 4.0 Hz, 1H), 3.67 (dd, *J* 11.0, 4.0 Hz, 1H), 3.88 (s, 3H), 4.75-4.80 (m, 1H), 7.15 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 4.2, 52.8, 53.7, 115.5 (q, *J* 286), 156.7 (q, *J* 35), 168.4; $[\alpha]_D^{22}$ +64.6 (c 0.99, $CHCl_3$); *m/z* (ES) Found: MH^+ 325.9510. $C_6H_8F_3INO_3$ requires MH^+ 325.9501.

^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (100 MHz, $CDCl_3$):



References

1 C. M. L. Goddard, A. R. Massah and R. F. W. Jackson, *Tetrahedron*, **66**, 9175-9181.

2 A. Wlodawer, M. Li, A. Gustchina, Z. Dauter, K. Uchida, H. Oyama, N. E. Goldfarb, B. M. Dunn and K. Oda, *Biochemistry*, 2001, **40**, 15602-15611.

3 J. R. Ragains and J. D. Winkler, *Organic Letters*, 2006, **8**, 4437-4440.

4 R. Benhida, M. Devys, J.-L. Fourrey, F. Lecubin and J.-S. Sun, *Tetrahedron Letters*, 1998, **39**, 6167-6170.

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Gas-phase study of new organo-zinc reagents by IRMPD-Spectroscopy, computational modeling and Tandem-MS: Supplementary Information Calculations

Ahmad R. Massah,[1] Frank Dreiocker,[2] Richard F.W. Jackson,[1] Barry T. Pickup,[1] Jos Oomens,[3,4] Anthony J. H. M. Meijer,[1] and Mathias Schäfer[2]

[1] *Department of Chemistry, The University of Sheffield, Sheffield, S3 7HF, United Kingdom*
[2] *Department of Chemistry, University of Cologne, Greinstrasse 4, 50939 Köln, Germany*
[3] *FOM Institute for Plasma Physics Rijnhuizen, Edisonbaan 14, Nieuwegein 3439 MN, The Netherlands*
[4] *University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*

(Dated: February 25, 2011)

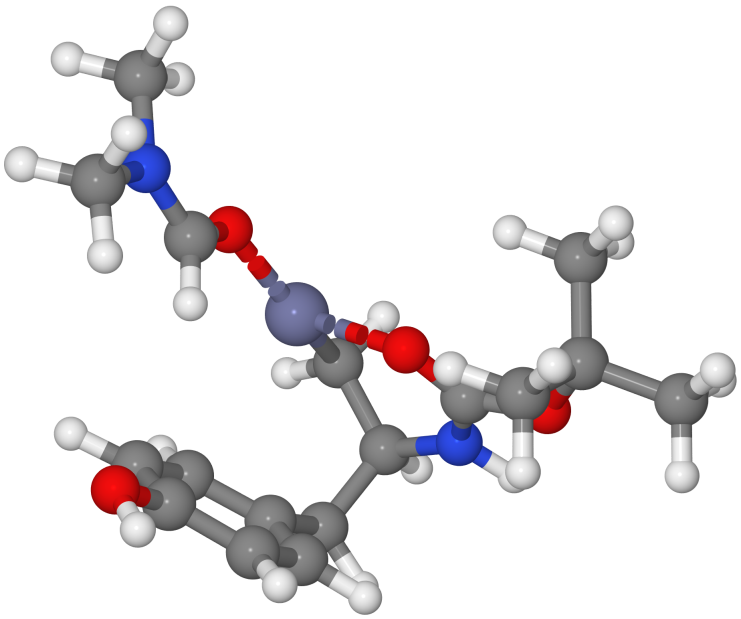
CONTENTS

NOTE

All calculations are presented in the order in which they are discussed in the main manuscript.

1. COMPOUND 1B [STRUCTURE FIG. 1(B)]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2ccc(cc2)O
Formula	:	$C_{17}H_{27}N_2O_4Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1301.78520803 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

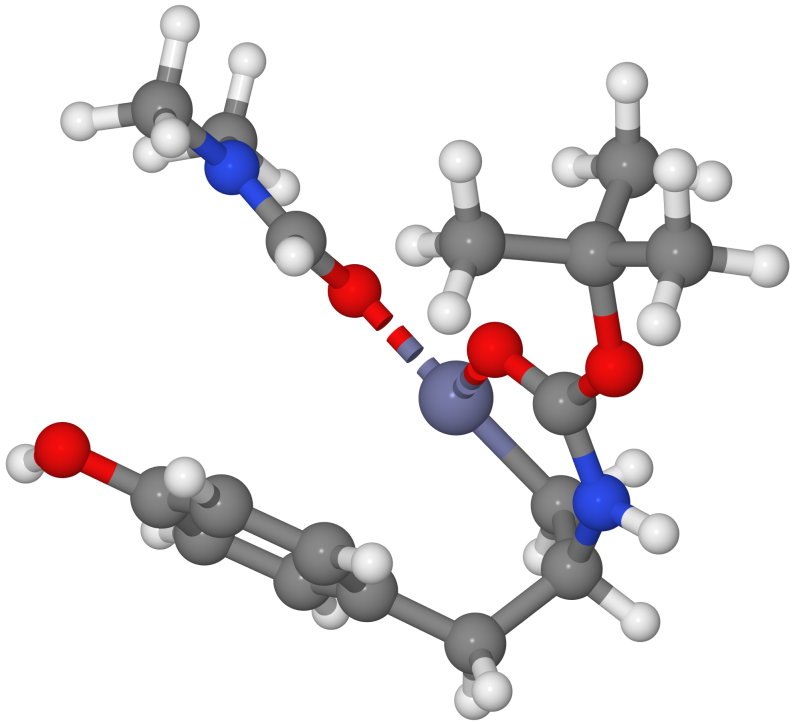
51

Zn	-0.64330733	-0.57221377	-1.28935874
C	0.48237291	-1.87689888	-2.21571946
H	-0.04833570	-2.78663206	-2.49845600
H	0.85208440	-1.41415918	-3.13454413
C	1.66515338	-2.23642325	-1.30736363
H	2.38355088	-2.81633615	-1.89628148
N	2.45351219	-1.05174243	-0.88149822
H	3.45723224	-1.16003716	-0.87513673
C	2.04269624	0.16356176	-0.46858242
O	0.85397738	0.54527348	-0.38444427
O	3.07773376	0.93075716	-0.15462762
C	2.96803546	2.36691689	0.25848737
C	1.29428494	-3.14507508	-0.09914881
H	0.86203009	-4.06058788	-0.51438928
H	2.22286344	-3.43815351	0.39840749
C	0.35099530	-2.54493785	0.91586769
C	0.83448273	-1.89306247	2.05542517
C	-1.04252362	-2.62203169	0.75626445
C	-0.02364182	-1.30700982	2.98089790
H	1.90374553	-1.84623110	2.23057437
C	-1.91513801	-2.04276848	1.67629778

H	-1.45656025	-3.19416642	-0.06740560
C	-1.40512896	-1.36607087	2.78620577
H	0.38155365	-0.80957127	3.85674000
H	-2.98878169	-2.14242291	1.56869638
C	2.20241237	2.46096706	1.57695246
H	2.23633194	3.49213266	1.93687439
H	1.16067576	2.16842866	1.45544708
H	2.66685772	1.82532537	2.33438873
C	4.43384123	2.75180244	0.44346270
H	4.98549891	2.63547873	-0.49114731
H	4.50473881	3.79477787	0.75870556
H	4.90475130	2.12790632	1.20544052
C	2.32368731	3.17637229	-0.86539704
H	2.85652852	3.01794267	-1.80576110
H	1.27521944	2.91519666	-1.00062072
H	2.38640261	4.23934269	-0.62052578
O	-2.30417585	-0.77752554	3.62928367
H	-1.86113310	-0.49653617	4.43778133
H	-3.90773153	1.78236198	-2.07356501
C	-4.48124313	2.17570615	-1.23909080
N	-3.86849046	1.73064756	0.01508813
H	-4.48752689	3.26728868	-1.27577746
H	-5.50982666	1.81228662	-1.29376209
C	-2.79664612	0.95721465	0.02503747
C	-4.49566603	2.16806674	1.26351070
O	-2.23121095	0.54075211	-1.01513362
H	-2.43046570	0.68899882	1.01959312
H	-4.46454382	3.25756526	1.33600092
H	-5.53756189	1.84153509	1.28733110
H	-3.97047305	1.73410249	2.11366606

2. COMPOUND 1B [STRUCTURE FIG. 1(B) WITH OH ROTATED]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2ccc(cc2)O
Formula	:	$C_{17}H_{27}N_2O_4Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1301.78407594 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

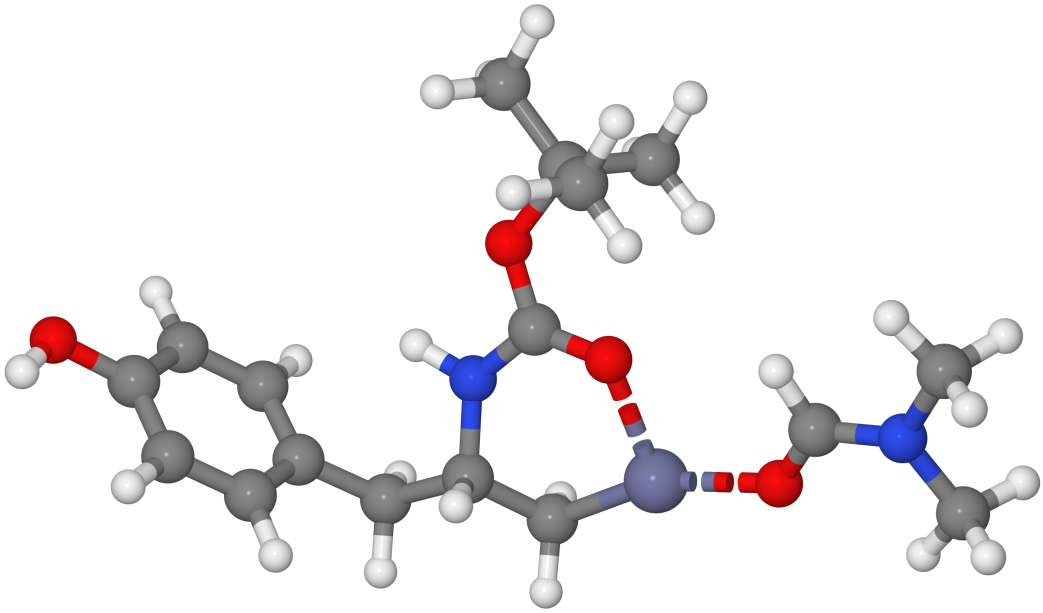
51

Zn	-0.34415901	-0.53918999	-1.56399202
C	0.70096600	-2.05378890	-2.21326709
H	0.08668800	-2.86337399	-2.60843801
H	1.35333502	-1.70931995	-3.01940799
C	1.54470694	-2.57492089	-1.04324102
H	2.25082803	-3.31582594	-1.43263495
N	2.43621802	-1.53807294	-0.45968899
H	3.37229896	-1.83559704	-0.22607601
C	2.20094609	-0.24200700	-0.17943700
O	1.12068498	0.36131001	-0.36872000
O	3.27968597	0.33201101	0.33667701
C	3.37868094	1.78202701	0.69644099
C	0.72606701	-3.31952000	0.04910800
H	0.30269200	-4.20715714	-0.43032801
H	1.42775702	-3.68271089	0.80541998
C	-0.38104299	-2.53977895	0.72439897
C	-0.13822500	-1.77488005	1.87551999

C	-1.69994700	-2.59247994	0.25140700
C	-1.15417397	-1.07934201	2.51731610
H	0.86260599	-1.74253201	2.29232597
C	-2.73264503	-1.90202796	0.88711703
H	-1.93779004	-3.21438503	-0.60508299
C	-2.46131992	-1.13901603	2.02368689
H	-0.96312302	-0.51280200	3.42067599
H	-3.74749708	-1.97819805	0.50882101
C	2.39512396	2.09497809	1.82252300
H	2.55732608	3.11933208	2.16630101
H	1.36303496	1.99923801	1.48847795
H	2.55805397	1.42638004	2.67074490
C	4.82210112	1.88682997	1.18300700
H	5.51878881	1.61418402	0.38831401
H	5.03442383	2.91246200	1.49157000
H	4.99181604	1.22733998	2.03607893
C	3.15480709	2.63705492	-0.54949498
H	3.82881403	2.32858896	-1.35178494
H	2.12728095	2.57263803	-0.90439600
H	3.37445498	3.68041396	-0.31094301
O	-3.41702390	-0.42902300	2.68855691
H	-4.29251289	-0.70148301	2.39236498
H	-3.45993090	2.04713607	-2.44334698
C	-3.70165396	2.79068303	-1.68926001
N	-2.80721092	2.61749792	-0.54141098
H	-3.57412410	3.79304910	-2.10388303
H	-4.73847103	2.66906095	-1.36787295
C	-1.88503599	1.67129302	-0.52208602
C	-2.97501397	3.53683805	0.58491498
O	-1.71012604	0.85481697	-1.46071398
H	-1.26745999	1.63817298	0.37944400
H	-2.80983305	4.56479502	0.25473100
H	-3.98714900	3.45167089	0.98610997
H	-2.26239991	3.29405308	1.37196803

3. COMPOUND 1B [STRUCTURE FIG. 1(C)]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2ccc(cc2)O
Formula	:	$C_{17}H_{27}N_2O_4Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1301.78499788 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

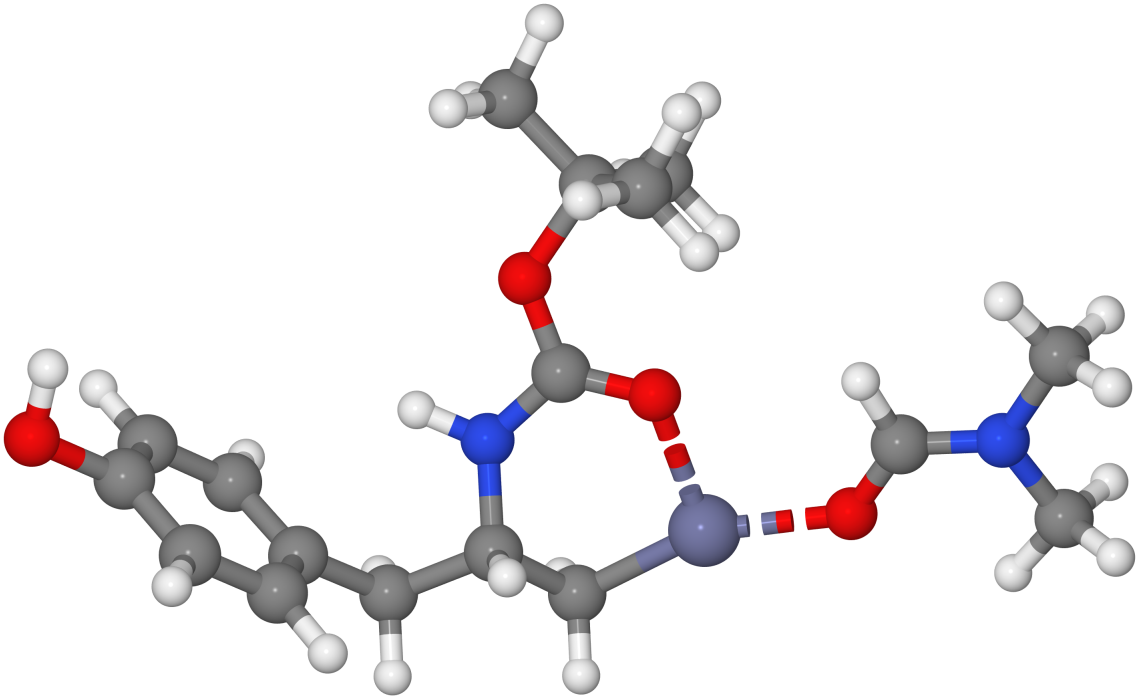
51

Zn	1.74906301	-1.53037786	-0.44145066
C	0.07497005	-2.36983252	-0.97890061
H	0.03217450	-3.41392565	-0.66490221
H	-0.01128931	-2.34680891	-2.06887650
C	-1.07994223	-1.59182167	-0.32934177
H	-1.03008056	-1.70992064	0.76030648
N	-1.04208910	-0.14050514	-0.62440389
H	-1.94266999	0.29631406	-0.78323901
C	-0.05517476	0.72554481	-0.34820095
O	1.11369753	0.40169895	-0.00942575
O	-0.45231703	1.97962356	-0.48826551
C	0.42905316	3.17872405	-0.33380690
C	-2.45397973	-2.12964416	-0.80210656
H	-2.47934365	-2.08736706	-1.89555633
H	-2.48706484	-3.18791890	-0.52920598
C	-3.65056014	-1.40109301	-0.23084815
C	-4.05018854	-1.59305644	1.09635937
C	-4.39002371	-0.50210601	-1.01148462
C	-5.13750839	-0.91065508	1.62982941
H	-3.51614785	-2.29915500	1.72462702
C	-5.47784901	0.18999512	-0.49172556

H	-4.12934017	-0.35804075	-2.05597067
C	-5.85699892	-0.01064983	0.83694845
H	-5.43555498	-1.08461571	2.65936160
H	-6.05406809	0.87420499	-1.10209656
C	1.55733216	3.12278414	-1.36223412
H	2.25328135	2.31086445	-1.15470862
H	1.15276551	2.99425554	-2.36859894
H	2.10861588	4.06579685	-1.34112966
C	0.92987198	3.25665903	1.10730326
H	1.47068799	4.19530487	1.24983752
H	0.08994547	3.24360657	1.80509257
H	1.59708905	2.42936087	1.34609663
C	-0.53654605	4.32066631	-0.64181662
H	-0.01746816	5.27735758	-0.55455220
H	-0.92990607	4.23161221	-1.65597522
H	-1.37444222	4.31636953	0.05738405
O	-6.92859888	0.68884730	1.29426849
H	-7.12145710	0.43977225	2.20448947
H	6.60993671	0.52656943	2.35924411
C	6.16464281	0.80302906	1.40121627
N	5.52506351	-0.36605394	0.79468358
H	5.42709446	1.58779359	1.56473207
H	6.94864750	1.18090427	0.74157715
C	4.23441601	-0.37605187	0.52030563
C	6.37845945	-1.52374446	0.50774199
O	3.64321470	-1.35797107	0.00158069
H	3.69012022	0.53826982	0.77370811
H	5.77450943	-2.30957985	0.06350653
H	6.82956743	-1.88239920	1.43534744
H	7.17089415	-1.22953963	-0.18367213

4. COMPOUND 1B [STRUCTURE FIG. 1(C) WITH ROTATED OH]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2ccc(cc2)O
Formula	:	$C_{17}H_{27}N_2O_4Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1301.78509881 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

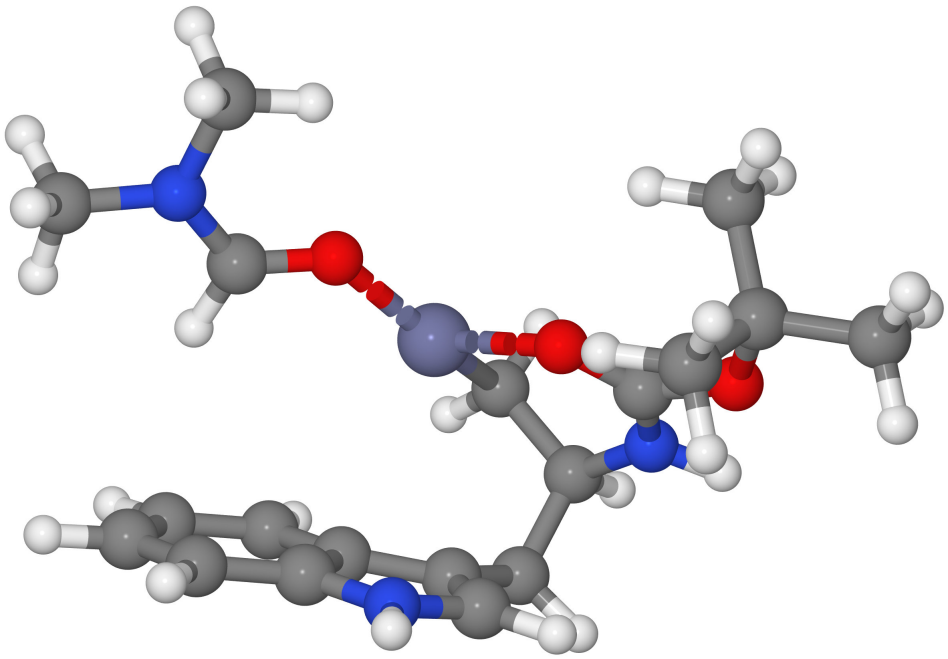
51

Zn	1.41533077	-1.52098846	-0.49146676
C	-0.30452698	-2.30138063	-0.97100514
H	-0.36161780	-3.35132408	-0.67953420
H	-0.44206026	-2.24891233	-2.05462599
C	-1.40332675	-1.50796652	-0.24710685
H	-1.29880667	-1.64915633	0.83579171
N	-1.34153199	-0.05252550	-0.51626623
H	-2.23686934	0.40934822	-0.62561184
C	-0.32030430	0.78060895	-0.26493636
O	0.85204792	0.41703904	0.01591420
O	-0.68739694	2.04803824	-0.36157274
C	0.23333120	3.21801615	-0.21407123
C	-2.81437182	-1.99827123	-0.65553391
H	-2.89811826	-1.93240952	-1.74491060
H	-2.86298323	-3.06100249	-0.40197772
C	-3.95672631	-1.24930263	-0.00450696
C	-4.23884296	-1.40369308	1.36138868
C	-4.76252413	-0.37690663	-0.74131078

C	-5.27472448	-0.71246505	1.96936214
H	-3.64787316	-2.09108877	1.95879233
C	-5.80838346	0.32601750	-0.14406371
H	-4.59285831	-0.25736859	-1.80716419
C	-6.06802177	0.16162106	1.21672988
H	-5.49842596	-0.84215814	3.02107573
H	-6.42707634	0.98906642	-0.74093008
C	1.31801891	3.15699267	-1.28812826
H	1.99830449	2.32143784	-1.12813616
H	0.87054646	3.06470180	-2.28022456
H	1.89622998	4.08373451	-1.26665938
C	0.79273927	3.24629021	1.20718050
H	1.36470711	4.16618633	1.35033524
H	-0.01881482	3.23805761	1.93783474
H	1.44570899	2.39572215	1.39885104
C	-0.71064502	4.39360094	-0.45552433
H	-0.16127107	5.33309317	-0.36704728
H	-1.14659703	4.34045839	-1.45471811
H	-1.51936710	4.39529324	0.27726975
O	-7.06875467	0.80919427	1.86924303
H	-7.57304001	1.34703755	1.24935126
H	6.42969227	0.30626586	2.19077492
C	5.95772839	0.63076282	1.26100183
N	5.26527262	-0.49733284	0.63518077
H	5.24805164	1.42728138	1.48119450
H	6.72730875	1.01351273	0.58734202
C	3.96568704	-0.46389535	0.40929899
C	6.07612181	-1.66469026	0.27366900
O	3.32973719	-1.40975189	-0.12341067
H	3.45578361	0.45354742	0.71709901
H	5.43545723	-2.41724777	-0.17670994
H	6.55069828	-2.06997252	1.16982901
H	6.85062265	-1.36465514	-0.43533519

5. COMPOUND 2B [STRUCTURE FIG. 2(A)]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2c[nH]c3c2cccc3
Formula	:	$C_{19}H_{28}N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1358.14607487 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

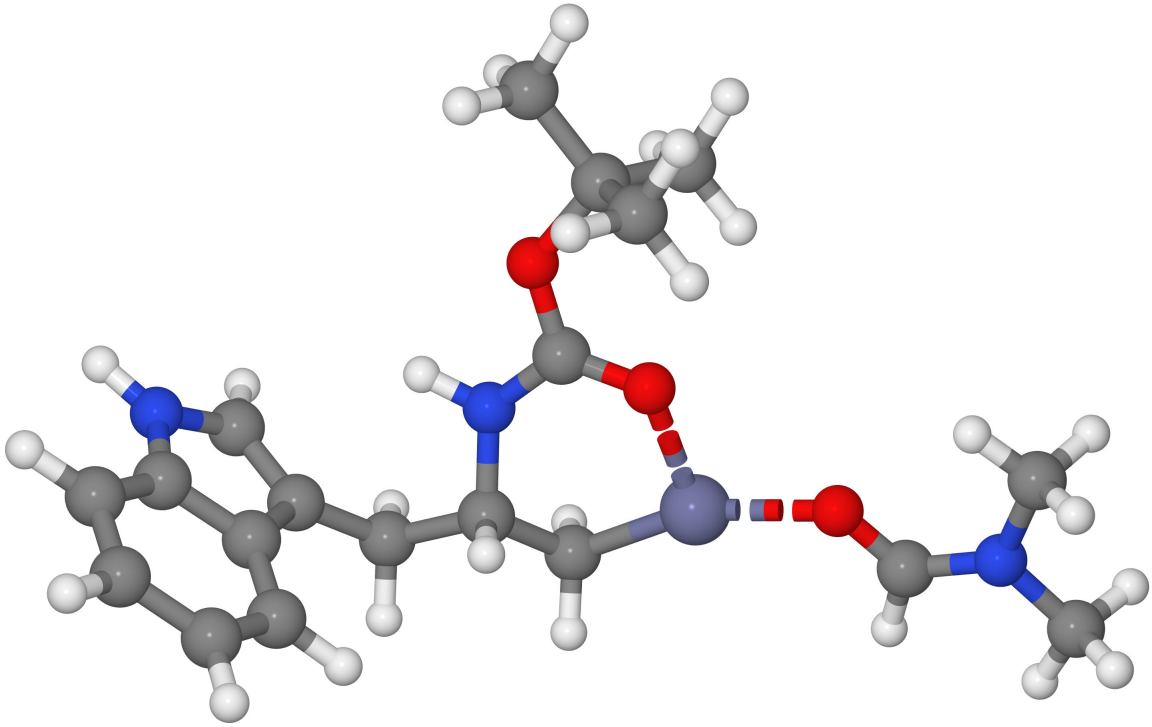
54

Zn	-0.21583664	0.14463209	-1.28257370
C	0.45356885	-1.23707163	-2.49473214
H	-0.33228794	-1.83897710	-2.95142841
H	1.00041974	-0.74413806	-3.30303574
C	1.40029562	-2.14990211	-1.70667171
H	1.91390073	-2.80898571	-2.41541433
N	2.51619887	-1.41392362	-1.05877936
H	3.41865325	-1.86611986	-1.07379472
C	2.51485538	-0.24053767	-0.39606643
O	1.52760386	0.50891435	-0.23232478
O	3.72379780	0.03902860	0.07451221
C	4.06882286	1.30668294	0.79491591
C	0.68249023	-3.09095979	-0.70118791
H	0.00889044	-3.72798300	-1.28366327
H	1.43570805	-3.76015997	-0.27504113
C	3.27829051	1.38272226	2.10011315
H	3.62597108	2.24179029	2.67898655
H	2.21133471	1.49729884	1.91528523
H	3.44611430	0.48504651	2.70022655

C	5.55994511	1.11785829	1.06301594
H	6.11169720	1.01618111	0.12670575
H	5.95072746	1.98332238	1.60197437
H	5.73476982	0.22632548	1.66828442
C	3.82125044	2.50313902	-0.12213957
H	4.33963346	2.36935186	-1.07441556
H	2.75934482	2.65274310	-0.31050748
H	4.21909428	3.40370107	0.35178721
C	-0.08190536	-2.43890333	0.41714531
C	-1.47610807	-2.04967618	0.43771809
C	0.40280911	-2.17055845	1.67450738
C	-1.75505579	-1.55142558	1.74339747
C	-2.53671503	-2.14215374	-0.48581854
H	1.38703763	-2.34969306	2.07930470
C	-3.03421760	-1.14396906	2.13237572
C	-3.80939674	-1.74701869	-0.09789050
H	-2.37247729	-2.54905081	-1.47680497
C	-4.05566597	-1.25250721	1.19922340
H	-3.23073530	-0.78955120	3.13798785
H	-4.63536119	-1.84931529	-0.79232067
H	-5.06584692	-0.97969043	1.48220468
N	-0.58507520	-1.62374508	2.46297646
H	-0.48384041	-1.39176536	3.43760729
H	-1.31765795	3.97271657	-0.36792475
C	-2.35972643	4.17777777	-0.13986146
N	-3.10999203	2.92023420	-0.16474259
H	-2.43927073	4.63255358	0.85013986
H	-2.77244735	4.86608458	-0.88092107
C	-2.52106428	1.76851082	-0.44135869
C	-4.54233265	2.98721933	0.12514566
O	-1.29538190	1.66544163	-0.69329792
H	-3.17609882	0.89256006	-0.42923924
H	-4.70106888	3.40764260	1.12076795
H	-5.04295540	3.62113619	-0.61025524
H	-4.97415924	1.98810709	0.08867552

6. COMPOUND 2B [STRUCTURE FIG. 2(B)]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn](O1)O[CH]N(C)C)Cc2c[nH]c3c2cccc3
Formula	:	$C_{19}H_{28}N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1358.14453478 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

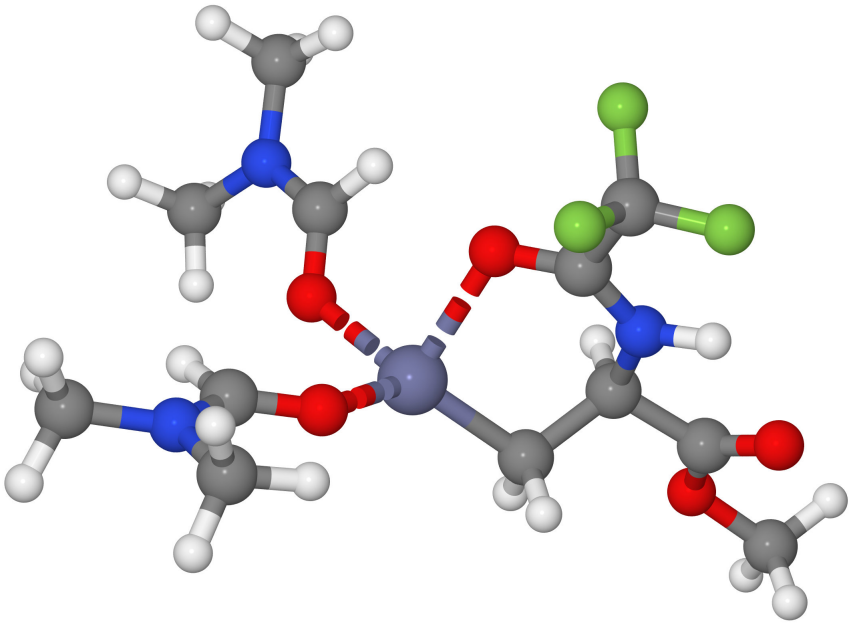
54

Zn	1.71266043	-1.62532878	-0.34270862
C	0.08080196	-2.58333731	-0.80465710
H	0.09258618	-3.60404921	-0.41906735
H	-0.01371799	-2.64042735	-1.89276779
C	-1.10775208	-1.82012928	-0.19914956
H	-1.04388213	-1.85364640	0.89569962
N	-1.14744246	-0.39317474	-0.59847128
H	-2.06681371	-0.01060865	-0.79106092
C	-0.20218232	0.53579807	-0.39402193
O	0.98308134	0.29456845	-0.04044203
O	-0.65842569	1.75675464	-0.62113678
C	0.16659959	3.00184965	-0.57166475
C	-2.45547104	-2.47060943	-0.60636568
H	-2.48208761	-2.54946160	-1.69832706
H	-2.43249464	-3.49531198	-0.22648634
C	1.28742766	2.91843653	-1.60665417

H	2.02281094	2.15830755	-1.34562731
H	0.88026327	2.69294000	-2.59475660
H	1.79379702	3.88476062	-1.66584098
C	0.67656815	3.21637249	0.85246605
H	1.17432356	4.18711042	0.91439503
H	-0.15561256	3.21963167	1.55959320
H	1.38343310	2.44155526	1.14684892
C	-0.85411584	4.07070017	-0.95563406
H	-0.37940669	5.05408716	-0.95161617
H	-1.25399196	3.88200831	-1.95337665
H	-1.68403578	4.08289242	-0.24714544
C	-3.68345165	-1.75960088	-0.11562142
C	-4.44264221	-0.75712204	-0.82661700
C	-4.29589319	-1.91499615	1.10409558
C	-5.49770069	-0.34471637	0.03143946
C	-4.35184336	-0.18503353	-2.10944557
H	-4.05226040	-2.58331895	1.91607916
C	-6.43750000	0.61555654	-0.34951171
C	-5.28306484	0.76924777	-2.48832035
H	-3.57860684	-0.49566275	-2.80465245
C	-6.31392813	1.16697586	-1.61583602
H	-7.23959351	0.91574591	0.31520584
H	-5.22790337	1.20976257	-3.47685242
H	-7.02979279	1.91120851	-1.94387627
N	-5.37625933	-1.06606519	1.19941235
H	-6.01285791	-1.02552640	1.97802913
H	7.11328888	-1.00669670	-0.15366234
H	6.81654787	-1.56751299	1.50807798
H	5.78182459	-2.14497066	0.17640185
H	3.54064250	0.62068957	0.71113741
O	3.59896421	-1.32345557	0.07093551
C	6.34178400	-1.29805577	0.56222719
C	4.13531256	-0.27642372	0.51605654
H	6.75689459	1.44430161	0.60695040
H	5.21836662	1.81899190	1.41361487
N	5.42486429	-0.17406268	0.77765989
C	5.99906445	1.06824863	1.29753458
H	6.46411276	0.88408583	2.26831174

7. COMPOUND 3A [STRUCTURE FIG. 3(B)]

General Information



SMILES	:	CN(C)[CH]O[Zn]1(CC(N[C](O1)C(F)(F)F)C(=O)OC)O[CH]N(C)C
Formula	:	$C_{12}H_{21}F_3N_3O_5Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1537.23534216 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

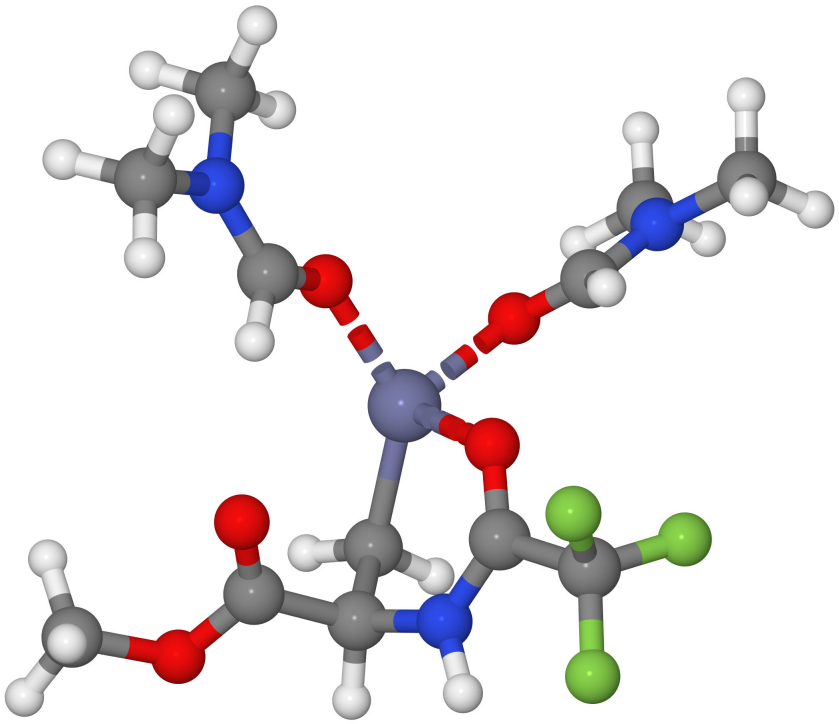
45

C	1.34319246	-0.60648590	1.34994829
N	2.39695024	-0.41535914	0.57840210
O	0.22424096	-0.07899858	1.21977806
C	1.52539575	-1.59769416	2.52146578
C	2.45310783	0.50515103	-0.56964588
H	3.26281977	-0.92157239	0.75772989
F	2.77745414	-2.08362484	2.58058548
F	1.25378370	-0.98312807	3.67709303
F	0.68037480	-2.62481833	2.37271643
C	1.39552152	0.21349739	-1.65104055
C	3.89215517	0.39407647	-1.08767569
H	2.32257462	1.52648950	-0.19618809
H	1.60111105	-0.75510055	-2.11542439
H	1.48930669	0.97341686	-2.42735338
Zn	-0.41409135	0.20961493	-0.84238267
O	4.69057560	-0.40845248	-0.66396976
O	4.12679672	1.28099775	-2.04661441
C	5.45362234	1.25712383	-2.63281655
H	5.45120907	2.05073667	-3.37444735
H	5.63724089	0.28930566	-3.09859347

H	6.20398808	1.44269657	-1.86480129
O	-1.81528687	-1.25380015	-1.06048667
C	-3.05954146	-1.20801127	-1.12952387
H	-3.59739470	-0.25664133	-1.05172563
N	-3.83337879	-2.27303076	-1.29982054
C	-5.28756094	-2.15398335	-1.37966406
C	-3.26165676	-3.61560750	-1.42045271
H	-5.64282084	-2.53079700	-2.34172702
H	-5.75647640	-2.73240733	-0.58006281
H	-5.58074093	-1.10922158	-1.27997112
H	-3.53775549	-4.04842472	-2.38483334
H	-2.18011165	-3.54600596	-1.34537947
H	-3.64668751	-4.25345421	-0.62142771
O	-1.76975536	1.67310476	-0.34223908
C	-1.83845639	2.21315813	0.78527236
N	-2.54869699	3.30284309	1.04525459
H	-1.29592872	1.79626274	1.63984931
C	-2.60335946	3.86848354	2.39317679
C	-3.30849934	3.98782063	-0.00150979
H	-2.22184491	4.89206982	2.38542414
H	-3.63458991	3.87919497	2.75378656
H	-1.99786758	3.26864171	3.07170701
H	-2.99624157	5.03305149	-0.05498913
H	-3.11853075	3.50032306	-0.95382112
H	-4.37652254	3.95040989	0.22741649

8. COMPOUND 3A [STRUCTURE FIG. 3(C)]

General Information



SMILES	:	CN(C)[CH]O[Zn]1(CC(N[C](O1)C(F)(F)F)C(=O)OC)O[CH]N(C)C
Formula	:	$C_{12}H_{21}F_3N_3O_5Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1537.23368624 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

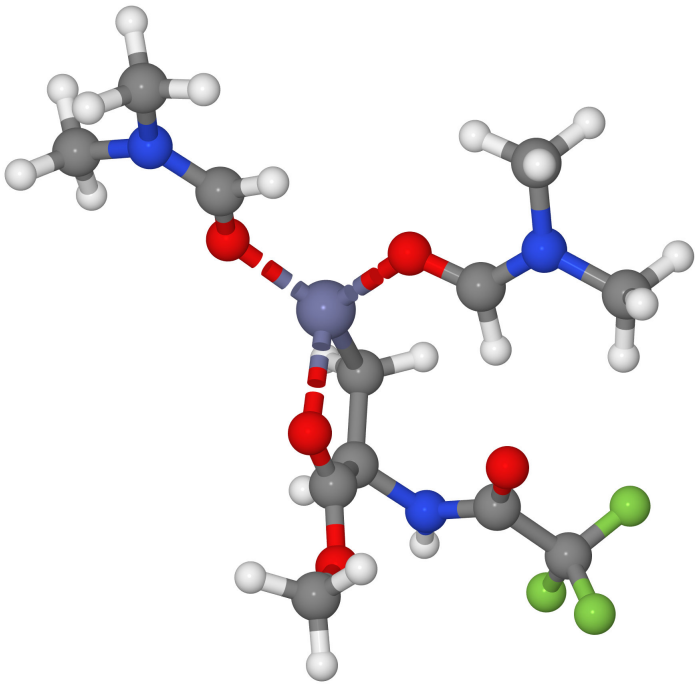
45

C	-0.29619774	-2.06077743	0.43111926
N	-1.22577035	-2.39485931	-0.46093625
O	0.32076669	-0.99718291	0.54534876
C	0.07545801	-3.17617631	1.44243550
C	-1.83264244	-1.56413949	-1.52684021
H	-1.61243010	-3.32322001	-0.35538027
F	-0.64458656	-4.30068445	1.24919069
F	1.37106788	-3.48207355	1.31158817
F	-0.14225280	-2.74769282	2.68689871
C	-0.83261573	-0.67898971	-2.29320788
C	-2.94099379	-0.69547564	-0.92200410
H	-2.30966258	-2.27977157	-2.20034814
H	-1.39959788	-0.09533633	-3.02151608
H	-0.16295727	-1.32668746	-2.86568284
Zn	0.24971327	0.44464010	-1.06713939
O	-2.83066607	-0.06631729	0.10562059
O	-4.01649237	-0.69435984	-1.70452487

C	-5.12049675	0.15155558	-1.29960835
H	-5.89559317	-0.01603433	-2.04181314
H	-4.80897045	1.19628620	-1.29670990
H	-5.46480227	-0.13383391	-0.30592409
O	-0.01849689	2.13074851	0.02606089
C	-0.89911753	2.34414148	0.88909906
H	-1.64802718	1.58577299	1.13385808
N	-1.00589466	3.48461819	1.56091142
C	-2.05376005	3.67694998	2.56124115
C	-0.08344138	4.59575081	1.32921171
H	-1.60862279	3.87539291	3.53931189
H	-2.68635750	4.52394485	2.28457046
H	-2.66976762	2.78082228	2.62745214
H	0.44705048	4.83605576	2.25394750
H	0.62817538	4.30692768	0.56050915
H	-0.64048076	5.47726727	1.00275147
O	2.27001047	0.72522491	-1.18937159
C	3.12274909	0.43574044	-0.32687730
N	4.42710209	0.64208990	-0.47289869
H	2.83536959	-0.02494451	0.62485260
C	5.37810755	0.26590332	0.57054025
C	4.96796513	1.24435949	-1.69198835
H	6.09008932	-0.46752736	0.18427688
H	5.92952967	1.14539552	0.91177434
H	4.84727383	-0.16941713	1.41674328
H	5.65742683	0.54755872	-2.17476988
H	4.14679575	1.47316825	-2.36571026
H	5.50782824	2.16105604	-1.44293344

9. COMPOUND 3A [STRUCTURE FIG. 6S]

General Information



SMILES	:	CN(C)[CH]O[Zn]1(CC([C](O1)OC)NC(=O)C(F)(F)F)O[CH]N(C)C
Formula	:	$C_{12}H_{21}F_3N_3O_5Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1537.23172245 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

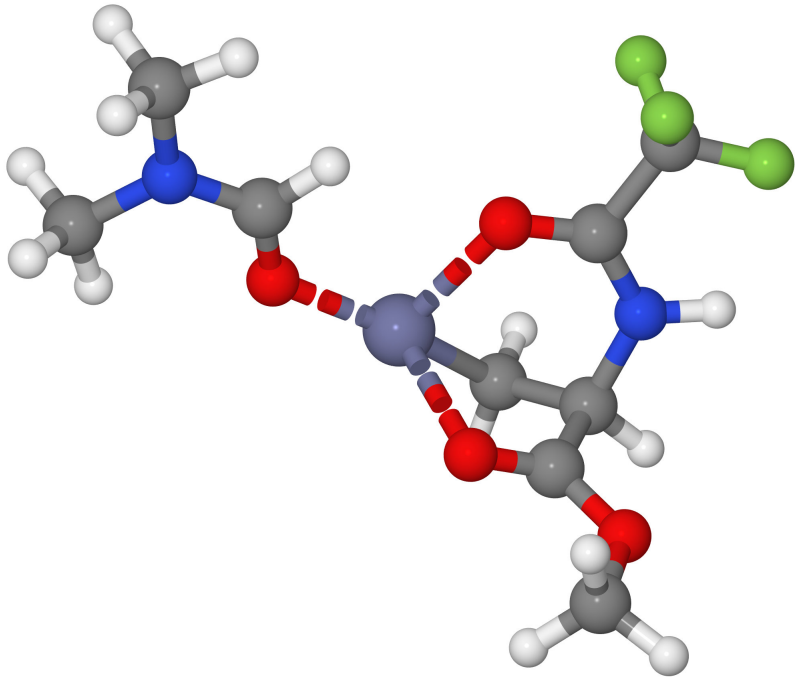
45

Zn	-1.20271301	-0.49183980	-0.73115796
C	0.40366346	-1.19770801	-1.65784287
H	0.16766353	-1.88666606	-2.46815825
H	0.93393016	-0.35244206	-2.09840870
C	1.30535841	-1.88985419	-0.61902547
H	1.28536367	-2.97276092	-0.77504492
N	2.71900845	-1.50346553	-0.69650531
C	0.81240475	-1.71891463	0.83586663
H	3.38978124	-2.13190579	-1.11224103
C	3.12008142	-0.29680446	-0.26729250
O	-0.28883091	-1.26866055	1.12724662
O	1.66032720	-2.18418837	1.72482908
O	2.39196229	0.53750187	0.24805751
C	4.62447071	0.01229203	-0.44880423
C	1.28266811	-2.09417272	3.12408638
F	4.77495193	1.10696983	-1.20208001
F	5.28003311	-1.00516069	-1.04994738

F	5.19274187	0.22934903	0.74085379
H	2.10516095	-2.54927325	3.66773915
H	1.16357684	-1.04810762	3.40358877
H	0.35321948	-2.63620234	3.29379869
O	-3.15891719	-0.91892344	-0.59295857
C	-4.06916237	-0.23021899	-0.08299956
H	-3.85521555	0.74890357	0.35630336
N	-5.33874226	-0.60884696	-0.03270484
C	-5.77284002	-1.89269829	-0.58745557
C	-6.36172438	0.23811513	0.57755482
H	-6.21491432	-2.50468087	0.20222811
H	-6.52040052	-1.72301495	-1.36575973
H	-4.91221142	-2.40356255	-1.00999677
H	-6.83586931	-0.28733557	1.40984631
H	-5.90901661	1.15616608	0.95083880
H	-7.12647629	0.49311480	-0.15987462
O	-1.44595230	1.49156046	-0.17469278
C	-0.44742140	2.18331265	0.14248924
N	-0.48437035	3.49199414	0.35654217
H	0.54167438	1.72963917	0.25901175
C	-1.71912801	4.26171064	0.22151528
C	0.72468847	4.21994495	0.74489915
H	-2.49702120	3.61650658	-0.17759454
H	-1.55448270	5.09971428	-0.45931727
H	-2.02713609	4.65365219	1.19451296
H	0.94376409	4.99829340	0.01025395
H	0.58348298	4.68709755	1.72259748
H	1.56716812	3.53134632	0.79634368

10. COMPOUND 3B [STRUCTURE FIG. 4]

General Information



SMILES	:	CN(C)[CH]O[Zn]12CC([C](O1)OC)N[C](O2)C(F)(F)F
Formula	:	$C_9H_{14}F_3N_2O_4Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1288.61530265 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

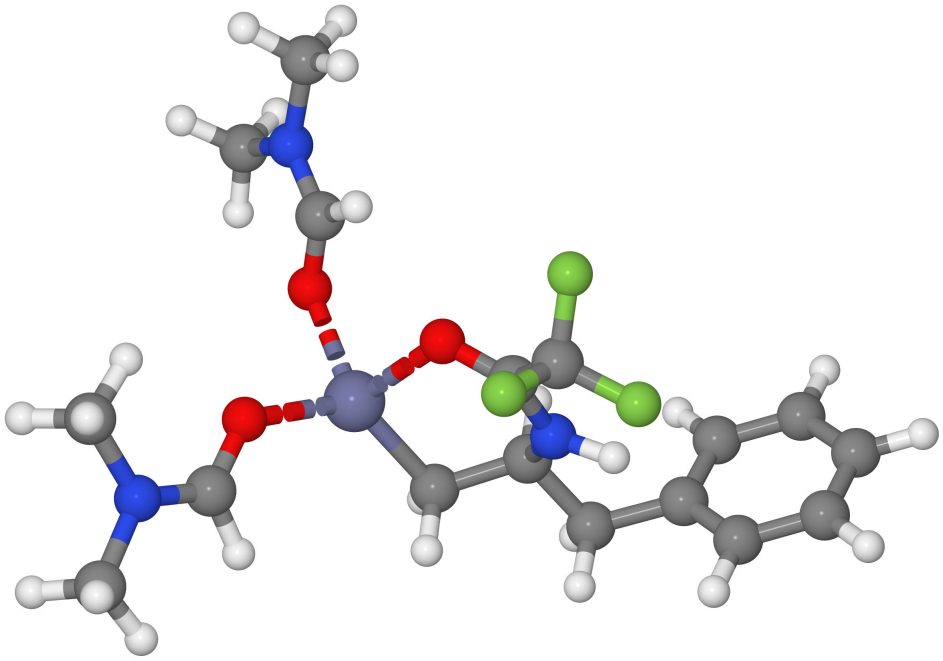
33

Zn	-0.61011058	-0.85915130	-1.01262712
C	1.04220498	-1.28058636	-1.99338663
H	1.04043341	-2.30087757	-2.37999320
H	1.26388168	-0.60459006	-2.81921339
C	2.10813260	-1.15939963	-0.90035230
H	3.08322120	-1.54670501	-1.20107019
N	2.35921693	0.24929464	-0.49409771
C	1.66075289	-1.93201482	0.35943878
H	3.31993699	0.56507432	-0.48353899
C	1.42852247	1.13745081	-0.14143805
O	0.48765364	-2.00254703	0.69391108
O	2.66067791	-2.46670890	1.01963794
O	0.21055165	0.94711715	-0.06343149
C	1.94930434	2.55599713	0.20121861
C	2.34643579	-3.20164776	2.23924184
F	1.43639362	3.43684363	-0.65881366
F	1.57305348	2.88295412	1.43820310
F	3.29376888	2.62167335	0.13132016
H	3.30202603	-3.57302332	2.59598470

H	1.89029562	-2.52937222	2.96465993
H	1.66759121	-4.02097702	2.00778627
O	-2.46531177	-0.61137813	-0.51219827
C	-2.93758798	0.30902839	0.20646860
N	-4.21734238	0.40985781	0.50816494
H	-2.29101491	1.08774042	0.62075853
C	-4.71554041	1.50377584	1.34491789
C	-5.20008039	-0.56252480	0.01947925
H	-5.45043087	2.08984208	0.78911620
H	-5.18910980	1.09823203	2.24142504
H	-3.89131594	2.15233016	1.63904297
H	-5.95195770	-0.04865637	-0.58316845
H	-4.69227982	-1.30978727	-0.58332002
H	-5.69087601	-1.04231775	0.86886358

11. COMPOUND 4A [STRUCTURE FIG. 5]

General Information



SMILES	:	CN(C)[CH]O[Zn]1(CC(N[C](O1)C(F)(F)F)Cc2ccccc2)O[CH]N(C)C
Formula	:	$C_{17}H_{25}F_3N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1579.72932123 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

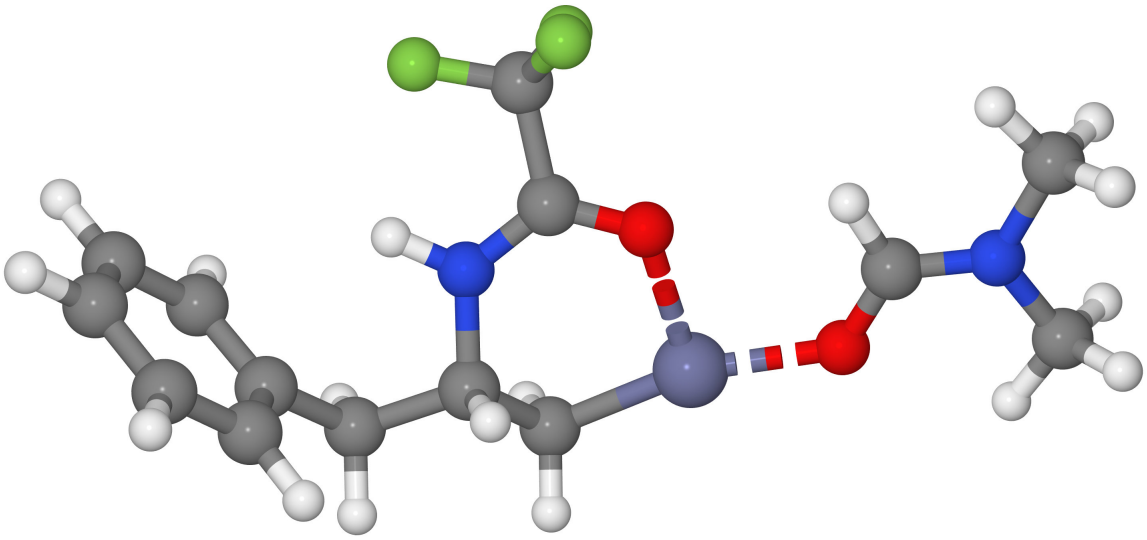
52

C	0.91404432	-0.34218204	0.77032065
N	1.78747749	-0.57774329	-0.19451346
O	-0.18862778	0.22214012	0.67386460
C	1.69058239	-0.12976553	-1.61295366
H	2.67991924	-0.97108525	0.08723742
C	0.36277580	-0.52658993	-2.27465463
C	2.91991234	-0.69675040	-2.36409926
H	1.77731049	0.96260160	-1.59234297
Zn	-1.17870176	0.15801612	-1.23597348
H	0.31858653	-1.61625755	-2.37531614
H	0.36047956	-0.11766358	-3.28797388
H	2.88101768	-0.28790328	-3.37705112
H	2.79732490	-1.78036487	-2.45858240
C	4.25308561	-0.38041553	-1.72050858
C	4.96572685	-1.36726308	-1.02927840
C	4.79007339	0.91207355	-1.78075624
C	6.17847824	-1.07068002	-0.40588978
H	4.58529520	-2.38437986	-1.00064731
C	6.00030851	1.20949459	-1.16259289

H	4.26482439	1.68767440	-2.32962775
C	6.69655609	0.21890658	-0.46968457
H	6.72008467	-1.84997487	0.11757119
H	6.40680122	2.21223927	-1.22778022
H	7.64126587	0.45073619	0.00769355
O	-2.04965067	1.97998750	-1.03035176
C	-2.13413262	2.62652421	0.03457373
H	-1.71800196	2.23517084	0.96886778
N	-2.71257424	3.81770444	0.13382709
C	-2.76994491	4.53004503	1.40853870
C	-3.31073928	4.47168493	-1.03056920
H	-2.25332212	5.48943138	1.32686663
H	-3.80968237	4.71334457	1.69013822
H	-2.29182649	3.93621397	2.18696356
H	-2.81135774	5.42560673	-1.21656311
H	-3.19733071	3.82378936	-1.89539683
H	-4.37127686	4.65795946	-0.84513503
O	-2.91570807	-0.83522308	-0.72597408
C	-3.28140092	-1.97162163	-1.08367085
N	-4.40448809	-2.55791020	-0.68426776
H	-2.68034387	-2.57683873	-1.77371860
C	-4.77273703	-3.89499712	-1.14551270
C	-5.32232714	-1.88828862	0.23748289
H	-4.00957441	-4.27788115	-1.82253063
H	-4.86414242	-4.57404518	-0.29444695
H	-5.72865868	-3.86017752	-1.67347801
H	-4.91951752	-0.90981996	0.48390761
H	-6.30215120	-1.77704656	-0.23302999
H	-5.43130207	-2.48263884	1.14781451
C	1.29962814	-0.85693902	2.17724252
F	0.44078615	-1.81422591	2.55221391
F	2.54315281	-1.37380183	2.20745969
F	1.23798072	0.14299594	3.06037784

12. COMPOUND 4B [STRUCTURE FIG. 6(B)]

General Information



SMILES	:	CN(C)[CH]O[Zn]1CC(N[C](O1)C(F)(F)F)Cc2ccccc2
Formula	:	$C_{14}H_{18}F_3N_2O_2Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1331.10752821 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

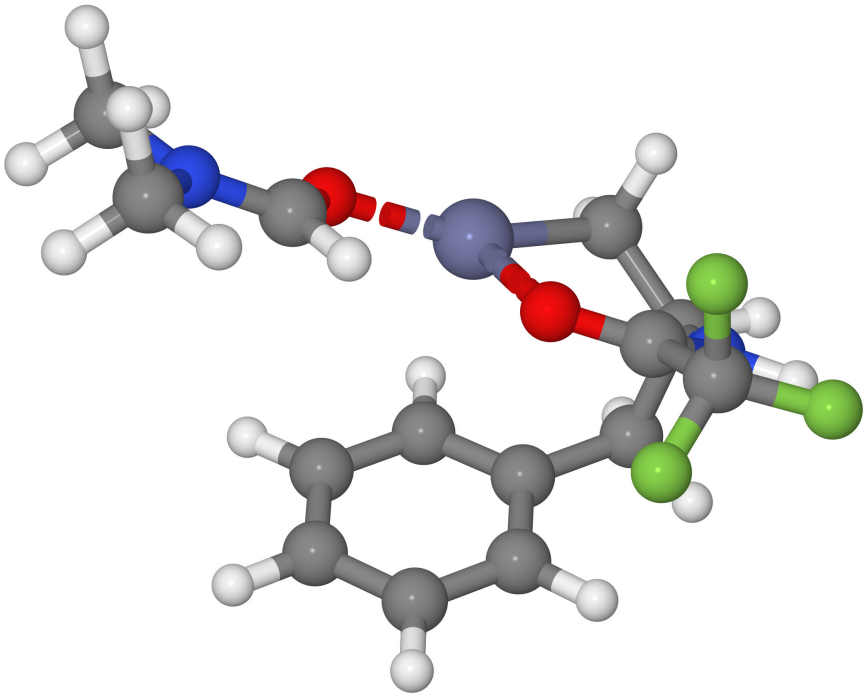
40

Zn	1.42324233	-1.69062388	-0.43460342
C	-0.32250389	-2.35768080	-0.99664021
H	-0.41736317	-3.42568827	-0.79533416
H	-0.42611280	-2.21948123	-2.07663107
C	-1.44159639	-1.61480141	-0.24942203
H	-1.36962771	-1.82046974	0.82421726
N	-1.35630369	-0.13357025	-0.39113522
H	-2.24126768	0.34341049	-0.54450327
C	-0.30461624	0.62847894	-0.16081297
O	0.84829038	0.25480121	0.14145400
C	-2.84526205	-2.05377817	-0.73379052
H	-2.88800478	-1.94057584	-1.82140076
H	-2.92803192	-3.12352729	-0.52535731
C	-3.98736596	-1.29908419	-0.08750445
C	-4.35281134	-1.55088055	1.24109173
C	-4.68381071	-0.31504121	-0.79939818
C	-5.38229513	-0.83386856	1.84215438
H	-3.84118485	-2.32550144	1.80406904
C	-5.71492100	0.40694991	-0.19682011
H	-4.44199705	-0.13152693	-1.84243083
C	-6.06359529	0.15012543	1.12533295
H	-5.66092396	-1.04793620	2.86741877
H	-6.25037193	1.15812266	-0.76549166

H	6.27971268	0.57158417	2.13356781
C	5.80933905	0.77918655	1.17035496
N	5.18300819	-0.44031149	0.65215659
H	5.05829906	1.55732059	1.29955721
H	6.57085800	1.12882781	0.47038338
C	3.89035892	-0.49062780	0.40758151
C	6.05673265	-1.59536278	0.41853192
O	3.30872345	-1.51937830	-0.03927390
H	3.32874203	0.42416981	0.61422741
H	5.46358919	-2.41987896	0.03404214
H	6.53252459	-1.88637400	1.35728824
H	6.82935190	-1.32528281	-0.30422673
H	-6.86839437	0.70426190	1.59345758
C	-0.51178658	2.15414739	-0.30614632
F	0.25956288	2.61042094	-1.29971182
F	-0.16119055	2.76504087	0.82704091
F	-1.79016232	2.46285534	-0.58307952

13. COMPOUND 4B [STRUCTURE FIG. 6(C)]

General Information



SMILES	:	CN(C)[CH]O[Zn]1CC(N[C](O1)C(F)(F)F)Cc2ccccc2
Formula	:	$C_{14}H_{18}F_3N_2O_2Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1331.10680015 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

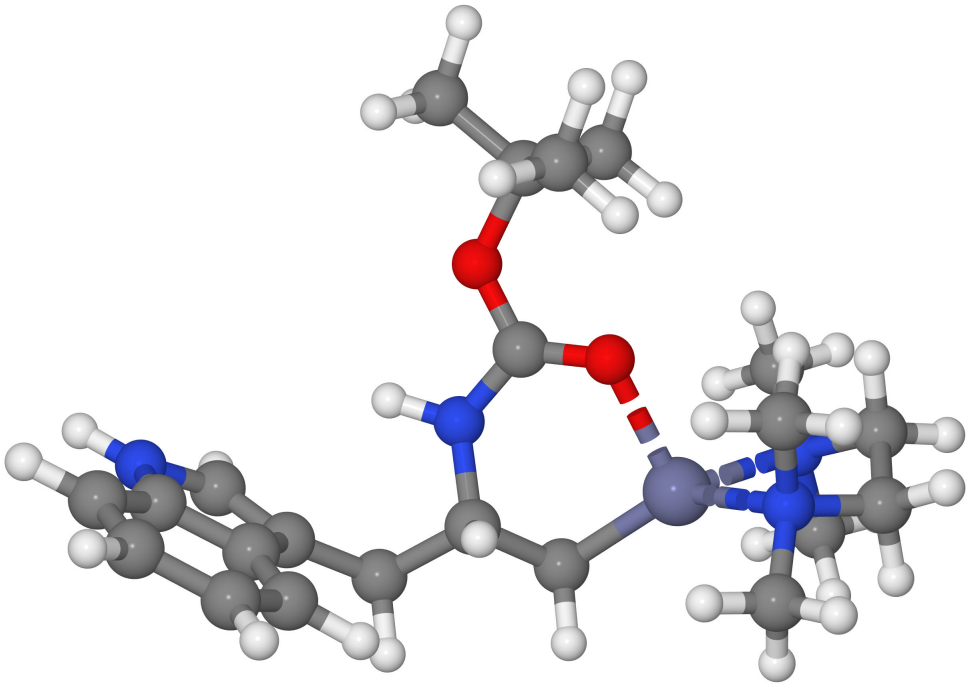
40

Zn	-0.77437121	-1.13589942	-1.08442342
C	0.54989904	-2.35658908	-1.85279191
H	0.16034670	-3.36201167	-2.01602435
H	0.85346150	-1.96410096	-2.82688975
C	1.76651192	-2.44278932	-0.92528135
H	2.55539966	-3.00913548	-1.43020391
N	2.40390348	-1.11103618	-0.68284690
H	3.41566563	-1.10572708	-0.66240102
C	1.82896137	0.06376283	-0.46586555
O	0.61712611	0.33365563	-0.42737952
C	1.50763261	-3.17421293	0.42213142
H	1.18249726	-4.18659735	0.16560392
H	2.46212721	-3.27668858	0.94539374
C	0.49886972	-2.52074814	1.33854878
C	0.91171253	-1.64244151	2.34683275
C	-0.87667120	-2.78181839	1.20687461
C	-0.01415585	-1.02910149	3.18750238
H	1.96998358	-1.45214438	2.49164534

C	-1.80632150	-2.16860771	2.05200958
H	-1.21482968	-3.52950907	0.49633351
C	-1.37634420	-1.28476942	3.03863430
H	0.33035466	-0.36358917	3.97044349
H	-2.85912538	-2.40721130	1.95408487
H	-4.67446327	0.26723319	-1.25135791
C	-4.82805395	1.28887105	-0.91612208
N	-3.54589677	1.84851193	-0.47786283
H	-5.22729301	1.89098573	-1.73507237
H	-5.53660822	1.30432010	-0.08517035
C	-2.43299031	1.14095116	-0.51807338
C	-3.54714775	3.23304701	-0.00050538
O	-2.38298154	-0.05066799	-0.92304164
H	-1.53138566	1.65586674	-0.17528379
H	-3.89742947	3.89799523	-0.79278111
H	-4.21117020	3.32759643	0.86131155
H	-2.53966165	3.52656531	0.29149857
H	-2.09333253	-0.82323259	3.70736146
C	2.79564285	1.25061965	-0.22733113
F	2.59290361	1.74741459	0.99666929
F	4.08693838	0.87552023	-0.32263744
F	2.56534863	2.20757437	-1.12735295

14. COMPOUND 2C [STRUCTURE FIG. 7]

General Information



SMILES	:	CC(C)(C)O[C]1NC(C[Zn]2(O1)[N](CC[N]2(C)C)(C)C)Cc3c[nH]c4c3cccc4
Formula	:	$C_{22}H_{37}N_4O_2Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1457.42719334 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

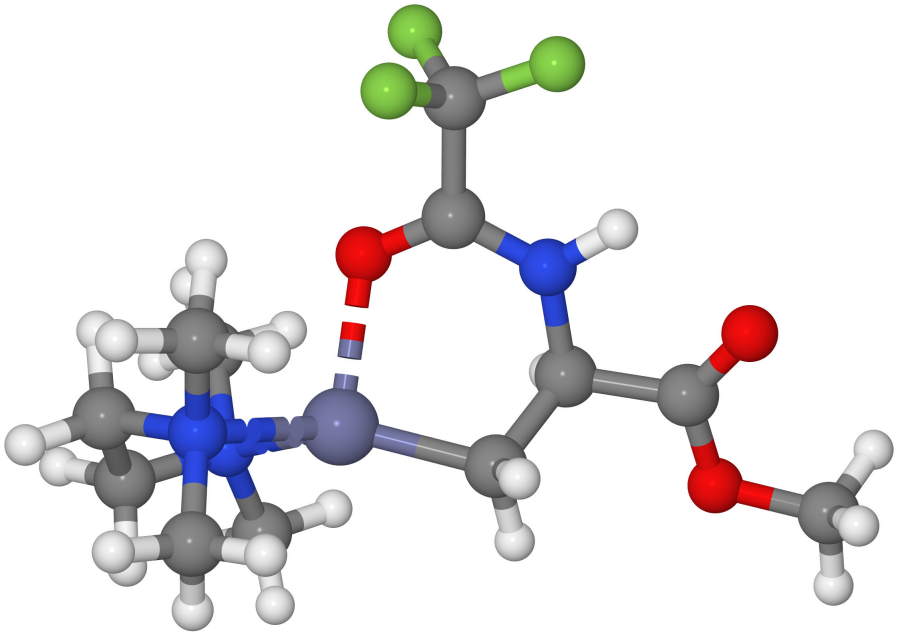
66

C	0.02402261	1.31055331	-0.20325319
Zn	1.96664011	-0.88344461	-0.36298740
C	-2.06534171	-1.34242451	-1.82828689
C	0.45797896	-1.55338466	-1.45565236
C	-0.85433793	-0.94657207	-0.94374925
C	0.24344876	3.66033626	0.63016993
N	-0.83065385	0.53264320	-0.88417619
O	1.11784267	0.93630606	0.28458244
O	-0.42608434	2.55908895	-0.11933232
H	0.59950668	-1.28518033	-2.50850821
H	0.37123898	-2.64265299	-1.41747820
H	-1.05043042	-1.31177664	0.07243734
H	-1.71663439	0.97747159	-1.09883833
C	4.35769939	-1.66237628	1.16763735
H	4.95110083	-1.69007111	2.08998322
H	4.53734303	-2.60516095	0.64761871
C	4.80968332	-0.48924807	0.30029854
H	4.68456602	0.44926673	0.84357375

H	5.87882757	-0.58897209	0.07293729
N	2.90484691	-1.58428490	1.47920251
N	4.01010370	-0.39634761	-0.94916177
C	2.38410378	-2.92319274	1.84890723
H	2.89949465	-3.32009673	2.73196983
H	1.31937933	-2.84923863	2.07126832
H	2.51724505	-3.61702728	1.01827276
C	2.65375590	-0.63935536	2.59518957
H	1.58179760	-0.56434512	2.77253580
H	3.14694595	-0.98388362	3.51246142
H	3.01900697	0.35458776	2.34311247
C	4.12446356	0.95703906	-1.54098701
H	5.16425514	1.18895972	-1.80250597
H	3.51810408	1.00866413	-2.44585800
H	3.75767636	1.70039046	-0.83493096
C	4.45518589	-1.40092647	-1.94652236
H	3.82187700	-1.33673632	-2.83125305
H	5.49717426	-1.22524190	-2.24094939
H	4.36968040	-2.40978551	-1.54352129
H	-2.11522532	-2.43580747	-1.82137001
H	-1.84322858	-1.04799938	-2.85944843
C	-3.37968254	-0.75734842	-1.40299916
C	-4.13704443	-1.07738090	-0.21594146
C	-4.10393524	0.19745135	-2.07755184
C	-5.30816698	-0.27498549	-0.23783170
C	-3.95432186	-1.97691047	0.84808201
H	-3.89834094	0.67028666	-3.02635741
C	-6.27639198	-0.33917379	0.76718503
C	-4.91388226	-2.04539895	1.84553123
H	-3.08390141	-2.62326717	0.88417542
H	-5.97223282	1.13032770	-1.69009256
C	-6.06216192	-1.23144257	1.80651808
H	-7.16668558	0.27862304	0.73472494
H	-4.78762197	-2.74094629	2.66701770
H	-6.79609108	-1.30981803	2.59983397
N	-5.25658417	0.49348345	-1.38196385
C	-0.71585280	4.82662725	0.40092301
H	-0.34708464	5.71695805	0.91436285
H	-0.80262321	5.05157232	-0.66376525
H	-1.70850563	4.58979321	0.78782254
C	1.61313450	3.95275903	0.02029486
H	2.31186080	3.13992047	0.21063235
H	1.52737868	4.10909176	-1.05748999
H	2.01691389	4.86669445	0.46226558
C	0.31989446	3.29446745	2.11171937
H	-0.67180389	3.04493594	2.49544239
H	0.98859435	2.45123839	2.28009987
H	0.69409341	4.15145016	2.67682028

15. COMPOUND 3C [STRUCTURE FIG. 8(B)]

General Information



SMILES	:	C[N]1(CC[N]([Zn]12CC(N[C](O2)C(F)(F)F)C(=O)OC)(C)C)C
Formula	:	$C_{12}H_{23}F_3N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1387.89734940 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

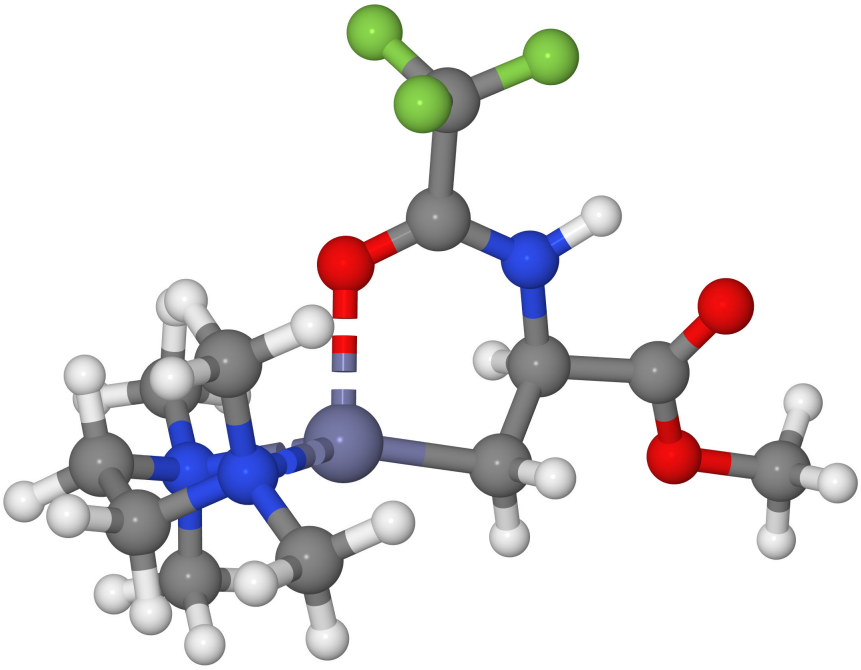
45

Zn	-0.92187649	-0.65440053	0.20355259
C	0.85257190	-1.40957940	0.69799930
C	1.93868458	-0.82044834	-0.22317608
H	1.09829748	-1.18306684	1.73992634
H	0.87976438	-2.49483275	0.59283900
C	3.35927820	-1.27529120	0.14119501
N	2.00272799	0.65046942	-0.20145044
H	1.75899231	-1.13941598	-1.25579989
O	4.23588800	-0.50968230	0.46577176
O	3.47896433	-2.59251499	0.04771708
C	0.99724752	1.46944046	-0.44066784
H	2.92393303	1.02614558	0.02216635
C	4.78147507	-3.14532661	0.37586376
O	-0.18196669	1.15271950	-0.68705451
C	1.32132375	2.98033094	-0.39478973
H	4.68174553	-4.21617937	0.22452125
H	5.03022957	-2.91904569	1.41217601
H	5.53992319	-2.72617745	-0.28445241
F	0.57562739	3.56066632	0.55683029
F	2.61478567	3.20890975	-0.11774949

F	1.02878129	3.54055810	-1.56944382
N	-2.55592728	0.14296158	1.35778642
C	-3.69375324	0.20469354	0.39888236
C	-2.25981450	1.49790466	1.89016831
C	-2.85810208	-0.76956254	2.49028850
C	-3.73085356	-1.02633798	-0.50342804
H	-3.56992841	1.10815597	-0.20072447
H	-4.64624691	0.30029240	0.93448532
H	-3.12998509	1.91113031	2.41325879
H	-1.42912233	1.43640101	2.59394455
H	-1.97834051	2.16161823	1.07424879
H	-1.99437761	-0.82190382	3.15321064
H	-3.72130442	-0.40902656	3.06199670
H	-3.07213163	-1.77580667	2.13021922
H	-4.56262684	-0.94087565	-1.21266246
H	-3.91121554	-1.92439830	0.09026115
N	-2.44151521	-1.21069098	-1.22866249
C	-2.29179358	-2.62386250	-1.65974832
C	-2.37847185	-0.32729000	-2.42298388
H	-3.10650921	-2.92109108	-2.33026505
H	-1.34569883	-2.74463439	-2.18776798
H	-2.29158473	-3.28164554	-0.78987336
H	-1.41913211	-0.45959443	-2.92206430
H	-3.18272138	-0.57412273	-3.12582684
H	-2.46024489	0.71809924	-2.13175821

16. COMPOUND 3C [STRUCTURE FIG. 8(C)]

General Information



SMILES	:	C[N]1(CC[N]([Zn]12CC(N[C](O2)C(F)(F)F)C(=O)OC)(C)C)C
Formula	:	$C_{12}H_{23}F_3N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1387.89730155 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

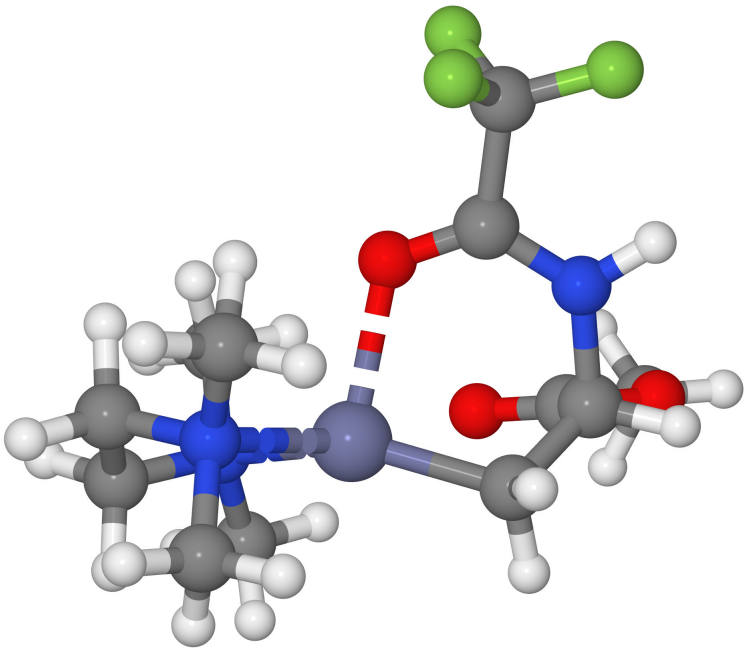
45

Zn	-0.91325939	-0.66171122	0.20059729
C	0.86855215	-1.39917088	0.69544381
C	1.94893575	-0.80432308	-0.22886431
H	1.11291206	-1.16724086	1.73646677
H	0.90457338	-2.48461485	0.59424567
C	3.37363052	-1.24293530	0.13880093
N	1.99769950	0.66721463	-0.21390660
H	1.77244544	-1.13013899	-1.25977433
O	4.24160290	-0.46707800	0.46229699
O	3.50725961	-2.55914664	0.04988484
C	0.98377293	1.47307467	-0.46152329
H	2.91371727	1.05402744	0.01201942
C	4.81490898	-3.09722447	0.38203689
O	-0.18943883	1.13990307	-0.71500826
C	1.28578210	2.98799396	-0.40572008
H	4.72660494	-4.16956615	0.23417342
H	5.05957842	-2.86485648	1.41797626
H	5.57004452	-2.67243552	-0.27847025
F	0.56124324	3.54128075	0.57883686

F	2.58339477	3.23365402	-0.16522631
F	0.94703513	3.56101680	-1.56093514
N	-2.56664419	0.08357967	1.37926257
C	-3.78076553	-0.45566708	0.70371228
C	-2.58717299	1.57020664	1.39096653
C	-2.49062896	-0.41244233	2.77717304
C	-3.62687683	-0.43950465	-0.81501907
H	-4.66925859	0.11831684	0.99226850
H	-3.93440461	-1.47697783	1.05715919
H	-3.45625854	1.93726039	1.94927156
H	-1.68026042	1.94337904	1.86545599
H	-2.61782670	1.96168065	0.37597898
H	-1.59699893	-0.01211440	3.25617743
H	-3.36783004	-0.09981856	3.35546398
H	-2.43147230	-1.50145268	2.78445315
H	-3.52285051	0.58662641	-1.17184210
H	-4.52683258	-0.85541433	-1.28424656
N	-2.41501307	-1.19062686	-1.24789262
C	-2.65737796	-2.65583467	-1.22384274
C	-2.02445698	-0.78216296	-2.62182379
H	-3.45443034	-2.93121958	-1.92440569
H	-1.74403524	-3.17911458	-1.50725663
H	-2.94099665	-2.98422265	-0.22402613
H	-1.14941263	-1.35320270	-2.93373775
H	-2.83678842	-0.97365320	-3.33250976
H	-1.77243710	0.27722844	-2.63325071

17. COMPOUND 3C [STRUCTURE FIG. 8(D)]

General Information



SMILES	:	C[N]1(CC[N]([Zn]12CC(N[C](O2)C(F)(F)F)C(=O)OC)(C)C)C
Formula	:	$C_{12}H_{23}F_3N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1387.89699613 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

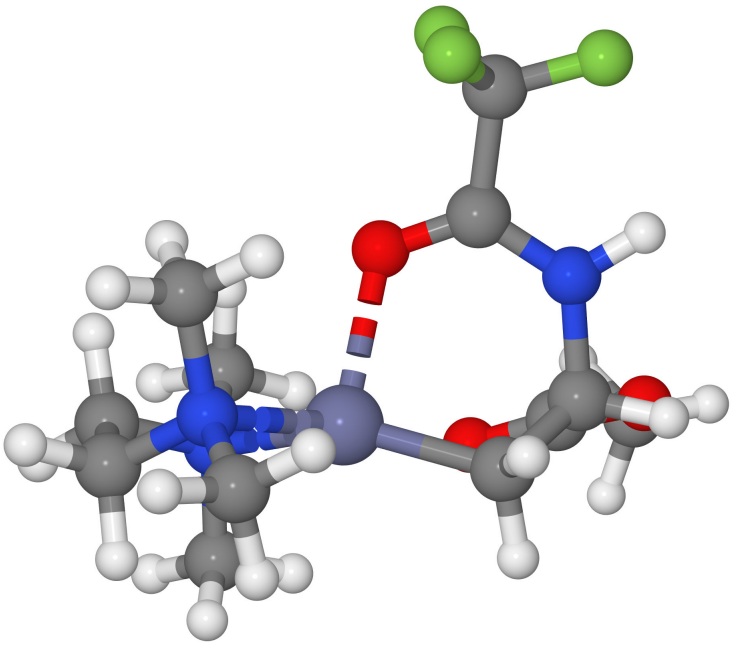
45

Zn	-0.96071261	0.30748966	-0.52248722
C	0.29228383	0.70722741	-2.01633072
C	1.72059107	0.82376194	-1.48100269
H	0.26822937	-0.07766429	-2.77733469
H	0.04648991	1.64371741	-2.52295113
C	1.85887480	1.96877444	-0.46112710
N	2.21349764	-0.41845274	-0.82430881
H	2.44481111	1.01329887	-2.27590704
O	1.02020776	2.23256779	0.37209758
O	3.01660681	2.60191774	-0.59956855
C	1.57229698	-1.15486765	0.08058878
H	3.15338159	-0.71181792	-1.05562758
C	3.28744411	3.69020772	0.32264918
O	0.43883038	-0.97621387	0.53931105
C	2.34536672	-2.39384007	0.60044748
H	4.26616383	4.06584167	0.03921149
H	3.29453492	3.31731462	1.34654474
H	2.52847004	4.46456003	0.21566540
F	1.66851878	-3.50232530	0.28270563
F	3.57778168	-2.48049545	0.06088707

F	2.46802115	-2.32544971	1.92573905
N	-2.09275651	1.23620963	1.03020871
C	-3.44046664	0.60108578	1.00494349
C	-2.21108961	2.70173383	0.80934888
C	-1.42026615	0.99939835	2.33660412
H	-3.95123124	0.74816799	1.96375251
H	-4.03608656	1.11282957	0.24682990
C	-3.35260534	-0.88981730	0.68892789
H	-2.82622218	3.16444969	1.58992398
H	-1.21674466	3.14319301	0.82438457
H	-2.67044449	2.89392710	-0.16138373
H	-0.43008712	1.44969034	2.30992055
H	-2.00338149	1.44557858	3.15067530
H	-1.30700362	-0.06812176	2.51952600
H	-2.81526089	-1.41209757	1.48267615
H	-4.36199999	-1.31867266	0.64627856
N	-2.62053013	-1.12986159	-0.58179432
C	-2.15698957	-2.53629947	-0.65249586
C	-3.47455049	-0.83899140	-1.75884330
H	-3.00372529	-3.23267436	-0.61958009
H	-1.61696434	-2.69249916	-1.58711863
H	-1.48436892	-2.74538422	0.17787492
H	-2.89628029	-0.98800302	-2.67094731
H	-4.34908676	-1.50070572	-1.78334320
H	-3.81985974	0.19477078	-1.74164152

18. COMPOUND 3C [STRUCTURE FIG. 8(E)]

General Information



SMILES	:	C[N]1(CC[N]([Zn]12CC(N[C](O2)C(F)(F)F)C(=O)OC)(C)C)C
Formula	:	$C_{12}H_{23}F_3N_3O_3Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-1387.89617185 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

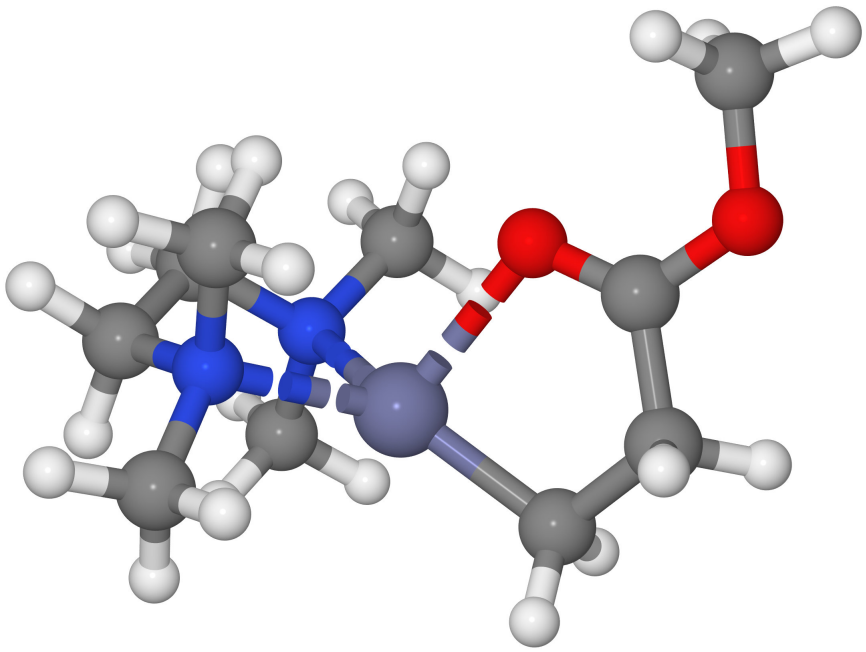
45

Zn	-0.96043634	0.27908835	-0.48500717
C	0.27231655	0.64472562	-2.00361991
C	1.70703983	0.78128606	-1.49823260
H	0.23657523	-0.16421011	-2.73879981
H	0.01424013	1.56424201	-2.53411770
C	1.86777246	1.97049391	-0.53185546
N	2.21344161	-0.43559799	-0.80377990
H	2.41865849	0.93813097	-2.31208062
O	1.00356424	2.34899330	0.22636783
O	3.08045602	2.50295353	-0.62758696
C	1.57842302	-1.16445804	0.11105074
H	3.16036677	-0.71802658	-1.01995099
C	3.38132691	3.61949492	0.25015429
O	0.44080660	-0.99438763	0.56509554
C	2.36405468	-2.38682508	0.65134495
H	4.39540815	3.91471505	-0.00260839
H	3.31664181	3.30282712	1.29096496
H	2.68191290	4.43449450	0.06701519
F	1.71919227	-3.50879455	0.31607115
F	3.61153102	-2.44697332	0.14327881

F	2.45145011	-2.31617093	1.97913754
N	-2.01742005	1.16236043	1.14261580
C	-3.18584585	0.27837759	1.41521621
C	-2.45869160	2.52129507	0.73036796
C	-1.17658710	1.27824831	2.36439490
H	-2.84335637	-0.52918279	2.06421089
H	-3.96009493	0.82581121	1.96576977
C	-3.77142167	-0.29586786	0.12844406
H	-3.02598929	3.00435090	1.53457141
H	-1.58084083	3.12294149	0.49887305
H	-3.08874321	2.46698093	-0.15806797
H	-0.33844265	1.93918467	2.15648770
H	-1.76382887	1.68259752	3.19710207
H	-0.79126364	0.29630646	2.63745284
H	-4.61065054	-0.96097267	0.36802623
H	-4.17019415	0.50667608	-0.49574956
N	-2.73575020	-1.01243651	-0.66077471
C	-2.47880483	-2.36416912	-0.10624428
C	-3.15711761	-1.13667393	-2.07630706
H	-3.38576412	-2.97998810	-0.14559987
H	-1.69716060	-2.85199475	-0.68820167
H	-2.13510513	-2.29957557	0.92481053
H	-2.37982750	-1.64939106	-2.64321280
H	-4.08950806	-1.70734525	-2.16555119
H	-3.30620265	-0.14685917	-2.50956011

19. COMPOUND 5 [STRUCTURE FIG. 10S]

General Information



SMILES	:	C[N]1(CC[N]([Zn]12CC[C](O2)OC)(C)C)C
Formula	:	$C_{10}H_{23}N_2O_2Zn^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-882.02169334 a.u.
Number of imaginary frequencies	:	0

Cartesian Co-ordinates (XYZ format)

38

Zn	0.22917713	-0.06827211	0.66269314
C	-1.03781593	-0.17217143	2.18789887
H	-1.02615786	0.78120047	2.72158337
H	-0.77830285	-0.94130886	2.91475701
C	-2.43235731	-0.43442011	1.59322786
H	-2.68519425	-1.50111473	1.64371741
H	-3.24124885	0.07596329	2.12378407
C	-2.54648709	-0.07508882	0.12670659
O	-1.57390261	0.09295366	-0.61663556
O	-3.78529859	0.01130442	-0.30200168
C	-4.00917435	0.29740825	-1.70709765
H	-3.56611919	-0.48492992	-2.32246733
H	-5.08880234	0.31406465	-1.82188225
H	-3.57783699	1.26442230	-1.96340370
N	1.54191005	-1.40967047	-0.41588059
C	2.71058536	-0.57471710	-0.81164950

C	0.84902501	-1.95223486	-1.61262786
C	1.97921181	-2.53608942	0.44760528
H	3.39099669	-0.52908504	0.04062924
H	3.26156187	-1.04615033	-1.63425684
C	2.27899337	0.83266717	-1.21785772
H	1.52047813	-2.60147643	-2.18686676
H	-0.01782830	-2.53254271	-1.29745936
H	0.49813575	-1.14379561	-2.25208712
H	1.11232674	-3.13132405	0.73489106
H	2.69153476	-3.18315792	-0.07742601
H	2.45078301	-2.15086174	1.35229433
H	3.16147304	1.43081582	-1.47636187
H	1.64839995	0.79103613	-2.10787439
N	1.49282706	1.49096954	-0.13926776
C	2.38083744	2.01070213	0.93169951
C	0.68817663	2.60893798	-0.69256067
H	3.05424166	2.78245211	0.54040724
H	1.77402163	2.44296002	1.72744524
H	2.98041677	1.20739019	1.35977364
H	0.12344297	3.08012676	0.11241156
H	1.33209097	3.36490393	-1.15723085
H	-0.01369658	2.22608733	-1.43258631