



# Strukturaufklärung komplexer Ionen in der Gasphase

Elektronischer Anhang

Katrin Peckelsen

aus Duisburg

Köln, 2018

# Inhalt

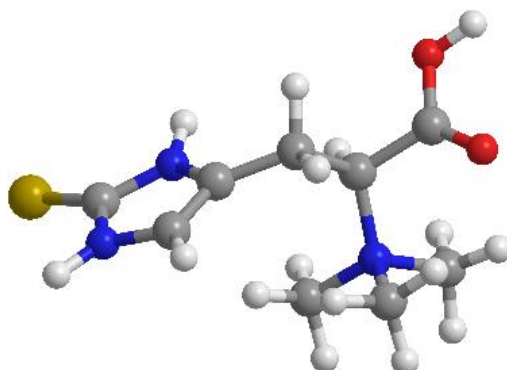
1 Ergothioneine .....	1
1.1 Thion a .....	1
1.2 Thion a2 .....	2
1.3 Thiol b .....	3
1.4 Thiol c .....	4
1.5 Thiol c2 .....	5
2 Ergothionein+Na <sup>+</sup> .....	6
2.1 Thiol a .....	6
2.2 Thiol b .....	7
2.3 Thion c .....	8
3 Hercynin .....	9
3.1 Konformer a .....	9
3.2 Konformer b .....	11
3.3 Konformer c .....	12
4 Hercynin+Na <sup>+</sup> .....	14
4.1 Konformer a .....	14
4.2 Konformer b .....	16
4.3 Konformer c .....	18
5 Nε-Methyl-Hercynin .....	20
5.1 Konformer a .....	20
5.2 Konformer b .....	22
5.3 Konformer c .....	24
6 Nε-Methyl-Hercynin+Na <sup>+</sup> .....	26
6.1 Konformer a .....	26
6.2 Konformer b .....	28
6.3 Konformer c .....	30
7 [Ni <sup>2+</sup> (His)(His-H)] <sup>+</sup> .....	32
7.1 Konformer a .....	32
7.2 Konformer b .....	34
7.3 Konformer c .....	36
8 [Ca <sup>2+</sup> (His)(His-H)] <sup>+</sup> .....	38
8.1 Konformer a .....	38
8.2 Konformer b .....	40

8.3	Konformer c.....	42
8.4	Konformer d.....	44
8.5	Konformer e.....	46
8.6	Konformer f.....	48
8.7	Konformer g.....	50
9	$[\text{Ni}^{2+}(\text{HisHis-H})]^+$ .....	52
9.1	a Im[NNNN] <sub>OH</sub> .....	52
9.2	b Im[NNNN].....	54
9.3	c Im[NNNNO].....	56
9.4	d Im[NNNO].....	58
9.5	e II[NNNO] <sub>OH</sub> .....	60
9.6	f CS[NNOO].....	62
10	$[\text{Ni}^{2+}(\text{HisHis-3H})]^-$ .....	64
10.1	a Im[NNNN] <sub>OH</sub> .....	64
10.2	b Im[NNNN] <sub>OH</sub> .....	66
10.3	c Im[NNNN].....	68
10.4	d Im[NNNN].....	70
10.5	e Im[NNNN].....	71
10.6	f Im[NNNN].....	73
11	$[\text{Ca}^{2+}(\text{HisHis-H})]^+$ .....	75
11.1	a CS[NNOO].....	75
11.2	b Im[NNNNO].....	77
11.3	c Im[NNNN].....	79
11.4	d Im[NNNN] <sub>OH</sub> .....	81
12	[pHis] <sup>-</sup> .....	83
12.1	Konformer a.....	83
12.2	Konformer b.....	84
12.3	Konformer c.....	85
13	$[\text{Ni}^{2+}(\text{pHis})]^-$ .....	86
13.1	Konformer a.....	86
13.2	Konformer b.....	87
14	[pHercynin] <sup>+</sup> .....	88
14.1	Konformer a.....	88
14.2	Konformer b.....	90

14.3 Konformer c.....	92
15 [pHisHis] <sup>-</sup> .....	94
15.1 Konformer a.....	94
15.2 Konformer b .....	96
15.3 Konformer c.....	97
16 NMR Spektren Hercynin und Nε-Methyl-Hercynin .....	99
17 Genehmigung zum Abdruck durch ACS.....	103

# 1 Ergothioneine

## 1.1 Thion a

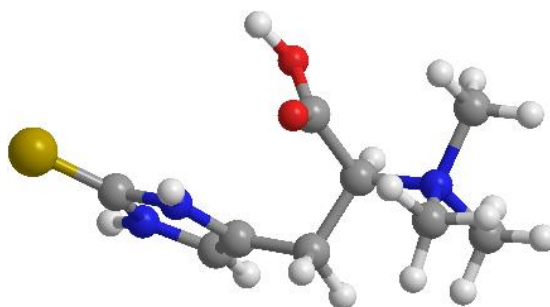


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      1.63108  0.16519  1.76661
C      0.90676 -0.53118  0.85595
C      3.00491 -0.20573 -0.026
N      2.88908  0.36612  1.22426
H      1.35489  0.52747  2.74265
N      1.74525 -0.7417  -0.23794
S      4.312   -0.23538 -1.04184
C     -0.51649 -0.95873  0.8724
H     -0.9556  -0.74045  1.847
H     -0.58012 -2.04594  0.7479
C     -1.42481 -0.3926  -0.25875
H     -1.01321 -0.66251 -1.2312
N     -1.58398  1.14099 -0.30796
C     -2.77928 -1.09238 -0.09107
O     -3.69114 -0.68024  0.57457
O     -2.75155 -2.26193 -0.73222
C     -0.32903  1.76891 -0.88383
H      0.51679  1.55035 -0.24323
H     -0.15963  1.37028 -1.88224
H     -0.4893  2.84404 -0.93648
C     -1.84909  1.73564  1.05629
H     -2.70897  1.23709  1.49399
H     -0.96114  1.6069  1.66946
H     -2.05095  2.79721  0.92459
C     -2.72567  1.50565 -1.23875
H     -2.68947  2.57917 -1.41178
H     -2.58859  0.97741 -2.1817
H     -3.66981  1.2332  -0.77936
H     -3.57413 -2.74694 -0.54994
H      3.67696  0.80344  1.67688
H      1.579   -1.35376 -1.02166
```

## 1.2 Thion a2

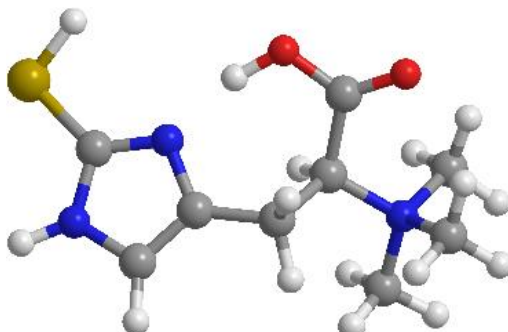


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

C	1.62242	1.93188	-0.48488
C	0.88733	1.10632	0.29947
C	2.97891	0.18435	0.09268
N	2.88134	1.37245	-0.59879
H	3.66855	1.75795	-1.09673
H	1.35333	2.85662	-0.96655
N	1.72248	0.04287	0.64419
S	4.27536	-0.8441	0.22402
C	-0.55891	1.13121	0.66683
H	-0.9207	2.15841	0.61153
H	-0.67984	0.78195	1.69487
C	-1.37123	0.22438	-0.29173
H	-1.304	0.61274	-1.30702
N	-2.88577	0.16619	0.01757
C	-0.77231	-1.19017	-0.26312
O	-0.2115	-1.48912	-1.42975
O	-0.78888	-1.89279	0.71521
C	-3.50872	1.49222	-0.34578
H	-3.05871	2.28196	0.2497
H	-3.351	1.68114	-1.40635
H	-4.57502	1.44124	-0.13254
C	-3.18284	-0.13602	1.47139
H	-2.64115	-1.03128	1.76272
H	-2.87767	0.71011	2.0813
H	-4.25695	-0.2855	1.56706
C	-3.51999	-0.90607	-0.84193
H	-4.60172	-0.83042	-0.74863
H	-3.22199	-0.75229	-1.87789
H	-3.18985	-1.88144	-0.49192
H	1.51618	-0.70439	1.28958
H	0.26349	-2.33521	-1.35541

### 1.3 Thiol b

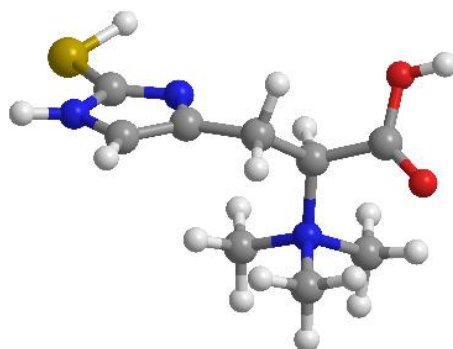


# opt freq b3lyp/cc-pvtz geom=connectivity empiricdispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
C      -1.82384  1.96416 -0.64385
C      -0.96729  0.89866 -0.58835
C      -2.89724  0.15325  0.06712
N      -3.04555  1.47085 -0.23479
H      -1.68666  2.99138 -0.93613
N      -1.64276 -0.21317 -0.13005
S      -4.22219 -0.81822  0.71101
C       0.4896  0.80759 -0.94025
H       0.89097  1.81905 -0.98751
H       0.61343  0.3813  -1.94047
C       1.26293 -0.07028  0.08751
H       0.74121 -0.03668  1.04588
N       2.67514  0.46138  0.41256
C       1.29017 -1.55214 -0.39626
O       2.31098 -2.09434 -0.74353
O       0.11942 -2.13913 -0.40899
C       2.55133  1.80799  1.08392
H       2.1032  2.52826  0.40637
H       1.93787  1.70445  1.97741
H       3.54858  2.14682  1.35756
C       3.53878  0.59969 -0.82232
H       3.63408 -0.37742 -1.28411
H       3.07313  1.30638 -1.50521
H       4.51119  0.97822 -0.51161
C       3.36512 -0.46171  1.40275
H       4.28609  0.02052  1.72478
H       2.70449 -0.60649  2.25655
H       3.57578 -1.40766  0.91833
H       -4.01497 -1.86425 -0.1151
H       -0.65448 -1.52121 -0.19271
H       -3.9172  1.97995 -0.20561
```

## 1.4 Thiol c



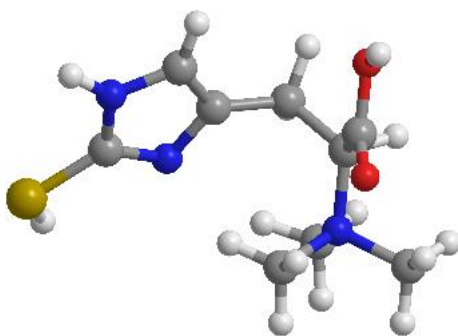
# opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      -1.8618  0.33777  1.92602
C      -0.94583  0.52621  0.92408
C      -2.82226  0.16933  -0.064
N      -3.06097  0.12022  1.2783
H      -1.78303  0.35844  3.00009
N      -1.54893  0.40495  -0.30811
S      -4.102  -0.15568  -1.24064
C      0.51293  0.86836  1.02042
H      0.93367  0.57247  1.98325
H      0.61865  1.95539  0.96747
C      1.35071  0.32547  -0.1607
H      0.73301  0.4218  -1.05589
N      1.71752  -1.17222  -0.08496
C      2.59487  1.20082  -0.34939
O      3.72937  0.90268  -0.08011
O      2.21928  2.38171  -0.84771
C      0.45485  -2.00827  -0.07641
H      -0.08843  -1.82846  0.84629
H      -0.16857  -1.72302  -0.92001
H      0.74879  -3.05408  -0.14291
C      2.52735  -1.52603  1.14245
H      3.43795  -0.93692  1.14926
H      1.9307  -1.3284  2.02899
H      2.75753  -2.58897  1.09303
C      2.50082  -1.55512  -1.32431
H      2.64185  -2.63412  -1.31766
H      1.92303  -1.26496  -2.2006
H      3.46331  -1.05487  -1.31264
H      3.00174  2.95199  -0.92366
H      -3.7653  0.86019  -2.06032
H      -3.96521  0.00752  1.71266
```



## 1.5 Thiol c2



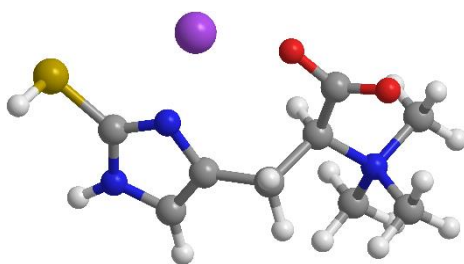
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

C	-1.06027	-1.04752	3.54929
C	-1.05351	-0.38549	2.35534
C	-1.92573	0.97873	3.77205
N	-1.61582	-0.15999	4.45144
H	-0.71228	-2.02056	3.84433
N	-1.60378	0.87159	2.50063
S	-2.6971	2.34061	4.56855
C	-0.5154	-0.81787	1.03132
H	-0.34218	-1.89185	0.99917
H	0.46088	-0.35111	0.88285
C	-1.35919	-0.34885	-0.16903
H	-0.7813	-0.54186	-1.0699
N	-1.67856	1.15308	-0.2122
C	-2.63284	-1.18876	-0.21048
O	-3.70271	-0.87438	0.24013
O	-2.36791	-2.36358	-0.78577
C	-0.53264	1.93672	0.37518
H	-0.45548	1.71813	1.43227
H	0.38682	1.64781	-0.1217
H	-0.74249	2.99045	0.21967
C	-2.93145	1.51303	0.54
H	-3.75592	0.93002	0.1498
H	-2.77694	1.3138	1.59415
H	-3.10829	2.57462	0.3954
C	-1.82259	1.58501	-1.64947
H	-1.91116	2.66643	-1.66907
H	-0.93251	1.27894	-2.19192
H	-2.7085	1.13114	-2.07451
H	-3.16221	-2.92047	-0.74113
H	-2.37159	3.20932	3.59637
H	-1.72196	-0.30814	5.44127

## 2 Ergothionein+Na<sup>+</sup>

### 2.1 Thiol a

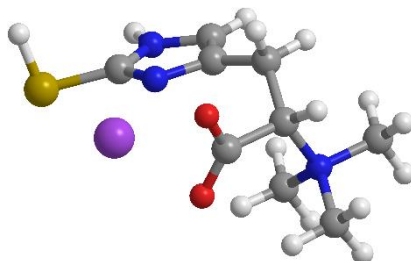


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

C	-1.39354	2.08301	-0.44755
C	-0.84223	0.83349	-0.60048
C	-2.90245	0.53651	0.0106
N	-2.69448	1.87858	-0.05226
H	-0.98996	3.07047	-0.59811
N	-1.79943	-0.11919	-0.3081
S	-4.41194	-0.21359	0.55304
C	0.55284	0.48093	-1.02912
H	0.98762	1.37074	-1.4855
H	0.50294	-0.26572	-1.82318
C	1.45582	-0.0744	0.11375
H	0.95316	0.06414	1.07161
N	2.77863	0.72563	0.28179
C	1.67058	-1.62803	-0.07628
O	2.79522	-2.06421	-0.30545
O	0.57263	-2.23253	0.01927
C	2.47445	2.15848	0.61808
H	1.96936	2.63926	-0.21491
H	1.84057	2.18874	1.50303
H	3.41076	2.67825	0.81608
C	3.63915	0.67024	-0.95871
H	3.84872	-0.37505	-1.16585
H	3.10306	1.12766	-1.78712
H	4.55372	1.22866	-0.76358
C	3.55994	0.14184	1.44101
H	4.44228	0.75916	1.60338
H	2.92627	0.15984	2.32677
H	3.83457	-0.87654	1.18711
H	-5.02772	-0.21778	-0.65114
H	-3.38353	2.58728	0.15321
Na	-1.50946	-2.45048	-0.05534

## 2.2 Thiol b

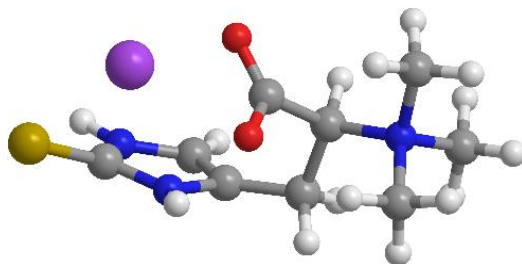


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      -1.09884 -2.22289 -0.59764
C      -0.53336 -0.99028 -0.82437
C      -2.48529 -0.62848  0.04241
N      -2.33096 -1.97809 -0.03944
H      -3.0111  -2.66456  0.25237
H      -0.74785 -3.22176 -0.79844
N      -1.4159  -0.00635 -0.41928
S      -3.88911  0.16698  0.77395
C       0.78612 -0.69705 -1.48444
H       0.58985 -0.12781 -2.39614
H       1.2402  -1.63694 -1.8036
C       1.80519  0.19607 -0.73416
H       2.59091  0.45437 -1.44515
N       2.5747  -0.48787  0.42607
C       1.08647  1.51902 -0.33979
O       0.83416  1.75029  0.86799
O       0.70952  2.17012 -1.33164
C       3.37023 -1.64785 -0.10647
H       2.69685 -2.42315 -0.46147
H       4.00631 -1.30364 -0.92062
H       3.9857  -2.0472  0.69818
C       1.67296 -0.98256  1.53215
H       1.08477 -0.13899  1.8793
H       1.02885 -1.76293  1.13775
H       2.30304 -1.3823  2.32582
C       3.54657  0.51762  1.0058
H       4.15254  0.01551  1.75845
H       4.18325  0.88846  0.2037
H       2.975  1.32833  1.44658
H      -4.65225  0.19891 -0.34226
Na     -1.20408  2.42848 -0.08551
```

## 2.3 Thion c



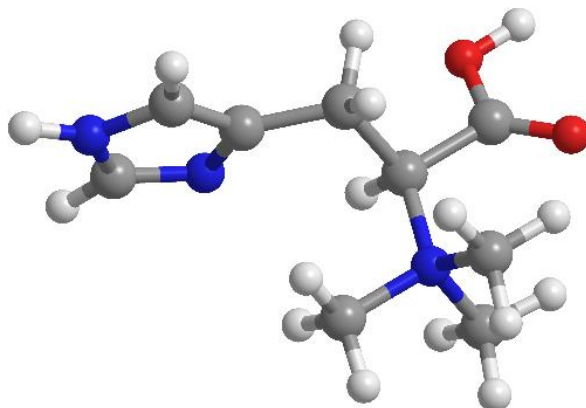
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      -1.30624 -2.2589 -0.68617
C      -0.55056 -1.57595 0.20947
C      -2.6294 -0.65389 0.22174
N      -2.57872 -1.70346 -0.6459
H      -3.36435 -1.96331 -1.22269
H      -1.05057 -3.06438 -1.35232
N      -1.40213 -0.65158 0.80547
S      -3.8581 0.49457 0.43384
C      0.92264 -1.50381 0.45151
H      1.38408 -2.45162 0.17082
H      1.09421 -1.3479 1.51797
C      1.52491 -0.32649 -0.3653
H      1.56566 -0.59635 -1.41977
N      2.99135 -0.00555 0.01425
C      0.61298 0.93818 -0.24175
O      -0.04094 1.2153 -1.26932
O      0.54118 1.48138 0.88429
C      3.88893 -1.11933 -0.45297
H      3.60337 -2.04648 0.03795
H      3.79613 -1.2219 -1.53296
H      4.91705 -0.87388 -0.19064
C      3.18983 0.2046 1.49887
H      2.42334 0.89356 1.84508
H      3.11144 -0.75167 2.0099
H      4.18839 0.61222 1.64831
C      3.38671 1.265 -0.70299
H      4.45839 1.41391 -0.5822
H      3.13404 1.16861 -1.75741
H      2.83931 2.09359 -0.26071
H      -1.10275 0.06479 1.45422
Na     -1.87113 2.29927 -0.45798
```

### 3 Hercynin

#### 3.1 Konformer a



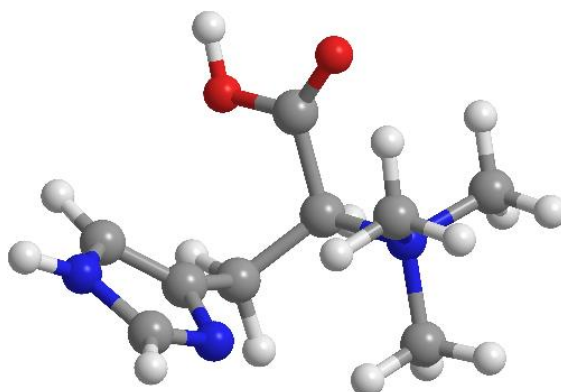
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

#### Kartesische Koordinaten (XYZ Format)

C	-2.94661	-0.78422	-0.83248
C	-1.75798	-0.50171	-0.20917
C	-3.29384	0.37704	1.01623
N	-3.9165	-0.21692	-0.03448
H	-4.91165	-0.24658	-0.19934
H	-3.18677	-1.33264	-1.72783
N	-1.98743	0.22481	0.93936
C	-0.36901	-0.94833	-0.58915
H	-0.17944	-0.82986	-1.65964
H	-0.28472	-2.02231	-0.41092
C	0.72828	-0.29456	0.25942
H	0.31623	-0.09307	1.24823
N	1.20986	1.09933	-0.24915
C	1.97621	-1.17437	0.467
O	3.09403	-0.79198	0.24671
O	1.67325	-2.40525	0.90056
C	0.04811	1.93288	-0.7392
H	-0.38489	1.47291	-1.62304
H	-0.69466	1.98973	0.05119
H	0.43329	2.92028	-0.98778
C	2.20179	0.94688	-1.37349
H	3.12038	0.51134	-0.98672
H	1.77596	0.30644	-2.14282
H	2.41232	1.93221	-1.78479
C	1.85543	1.85707	0.89384
H	2.22547	2.80456	0.50546
H	1.09589	2.03282	1.65336
H	2.66559	1.26564	1.30788

H	2.50168	-2.89203	1.04359
H	-3.8256	0.90068	1.79499

## 3.2 Konformer b

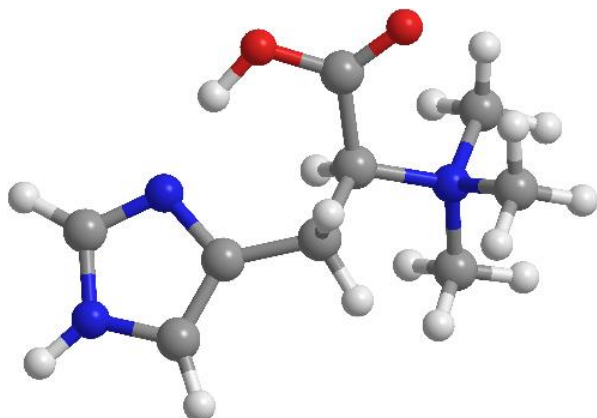


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      2.51813  0.89521  0.19271
C      1.54561 -0.00188  0.55606
C      3.00138 -1.12469 -0.56368
N      3.43894  0.16323 -0.52137
H      4.29723  0.51451 -0.9192
H      2.64183  1.94624  0.3918
N      1.8597  -1.25887  0.0765
C      0.3379  0.22231  1.40828
H      0.4546  1.15392  1.96224
H      0.27511 -0.56475  2.16018
C     -1.03488  0.36119  0.70363
H     -1.76392  0.54469  1.49889
N     -1.58172 -0.90061 -0.00495
C     -1.11072  1.6037  -0.19931
O     -1.62066  1.66615 -1.28594
O     -0.5681  2.65031  0.43372
C     -1.32347 -2.1116  0.86444
H     -0.25667 -2.32562  0.86087
H     -1.68479 -1.91386  1.87274
H     -1.87297 -2.94851  0.43775
C     -0.96748 -1.18159 -1.36768
H     -1.20785 -0.36746 -2.04024
H      0.10344 -1.30292 -1.24019
H     -1.40528 -2.11219 -1.72553
C     -3.07924 -0.75094 -0.1723
H     -3.45835 -1.64803 -0.65796
H     -3.53538 -0.64603  0.81124
H     -3.28239  0.11876 -0.78899
H     -0.68137  3.43483 -0.12725
H      3.54497 -1.91169 -1.06271
```

### 3.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

#### Kartesische Koordinaten (XYZ Format)

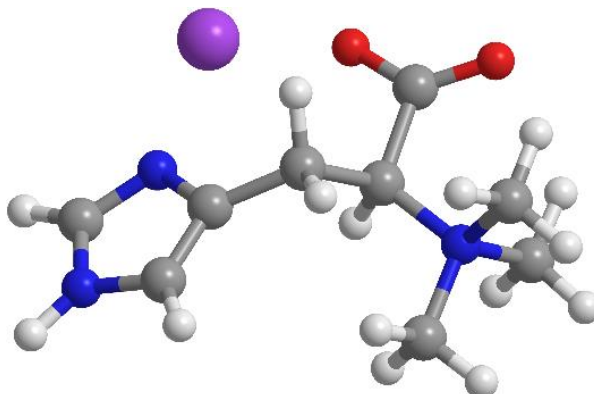
C	2.80708	-1.27376	-0.50659
C	1.75412	-0.40903	-0.37117
C	3.4357	0.5238	0.62389
N	3.86637	-0.6607	0.12883
H	2.90124	-2.23204	-0.9884
N	2.16143	0.70126	0.33847
C	0.34643	-0.51168	-0.88619
H	0.14173	-1.55765	-1.11104
H	0.24806	0.02989	-1.83205
C	-0.67279	0.06484	0.13867
H	-0.25769	-0.02935	1.14395
N	-1.99497	-0.72972	0.20501
C	-0.91214	1.57911	-0.14683
O	-1.97027	1.99397	-0.55352
O	0.12777	2.34339	0.07297
C	-1.70667	-2.12411	0.70662
H	-1.06918	-2.65372	0.00533
H	-1.21927	-2.05859	1.67798
H	-2.65149	-2.65545	0.80242
C	-2.68405	-0.81853	-1.13939
H	-2.90134	0.18862	-1.47916
H	-2.03037	-1.33087	-1.84137
H	-3.60123	-1.39067	-1.00951
C	-2.93927	-0.08835	1.20762
H	-3.7892	-0.75479	1.34149
H	-2.40967	0.03097	2.1519
H	-3.26136	0.8733	0.82641
H	0.97181	1.83448	0.31034



H	4.80235	-1.03012	0.21007
H	4.06528	1.20759	1.17012

## 4 Hercynin+Na<sup>+</sup>

### 4.1 Konformer a



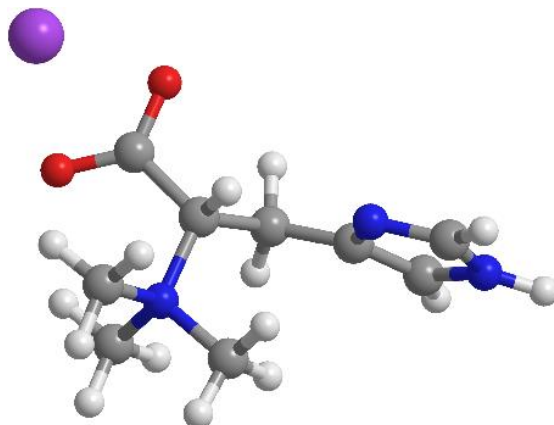
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

#### Kartesische Koordinaten (XYZ Format)

C	2.20628	-1.82322	-0.38354
C	1.57065	-0.61025	-0.43927
C	3.52112	-0.25457	0.43589
N	3.44186	-1.57984	0.17598
H	1.90634	-2.80747	-0.70122
N	2.41147	0.36797	0.07914
C	0.20166	-0.31211	-0.97912
H	-0.12245	-1.1782	-1.55687
H	0.2702	0.50827	-1.69461
C	-0.84862	0.0799	0.10262
H	-0.38902	0.00775	1.08937
N	-2.03682	-0.91795	0.1877
C	-1.28719	1.58745	-0.07963
O	-2.46447	1.8631	-0.28805
O	-0.28413	2.34168	0.01431
C	-1.5272	-2.30126	0.47975
H	-0.93738	-2.66571	-0.35637
H	-0.9136	-2.27149	1.37877
H	-2.37863	-2.9627	0.63352
C	-2.85273	-0.9391	-1.08351
H	-3.22607	0.06665	-1.2518
H	-2.22101	-1.25795	-1.90942
H	-3.668	-1.64945	-0.95289
C	-2.93792	-0.51127	1.33546
H	-3.73062	-1.25248	1.42626
H	-2.3438	-0.48998	2.24816
H	-3.34233	0.47158	1.11715
H	4.16479	-2.26304	0.346
Na	1.77586	2.66525	0.18799

H 4.39406 0.20338 0.87429

## 4.2 Konformer b



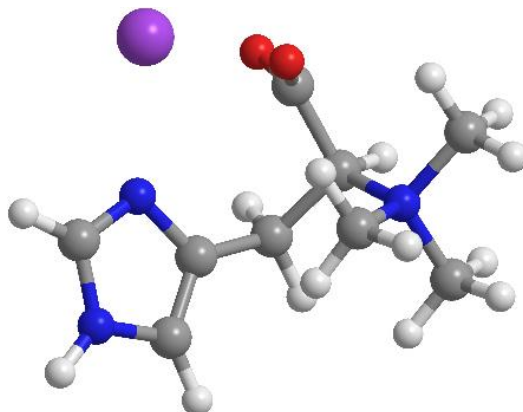
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

### Kartesische Koordinaten (XYZ Format)

C	3.12006	-0.85319	1.06086
C	1.97031	-0.63608	0.34429
C	3.57259	-0.64253	-1.09172
N	4.13521	-0.85842	0.12657
H	5.11525	-1.00408	0.31528
H	3.30286	-1.01995	2.10914
N	2.26735	-0.50164	-0.99443
C	0.54681	-0.61809	0.83535
H	0.48494	-0.19844	1.84327
H	0.19269	-1.64752	0.91146
C	-0.44617	0.05836	-0.12777
H	-0.06534	-0.10769	-1.13794
N	-0.50989	1.60458	0.00587
C	-1.83758	-0.63515	-0.074
O	-2.89651	0.04083	0.05561
O	-1.79173	-1.87784	-0.2031
C	0.87815	2.19382	-0.05856
H	1.44404	1.88896	0.81716
H	1.37613	1.82739	-0.9524
H	0.78291	3.27839	-0.08025
C	-1.15371	2.04217	1.29759
H	-2.1731	1.67213	1.31449
H	-0.58274	1.63904	2.13059
H	-1.1308	3.13035	1.33661
C	-1.29078	2.1713	-1.15832
H	-1.29476	3.25696	-1.07266
H	-0.79114	1.87554	-2.07959
H	-2.30037	1.77735	-1.1199
Na	-4.03727	-1.934	-0.11684
H	4.14858	-0.59371	-2.00257



### 4.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine  
pop=regular

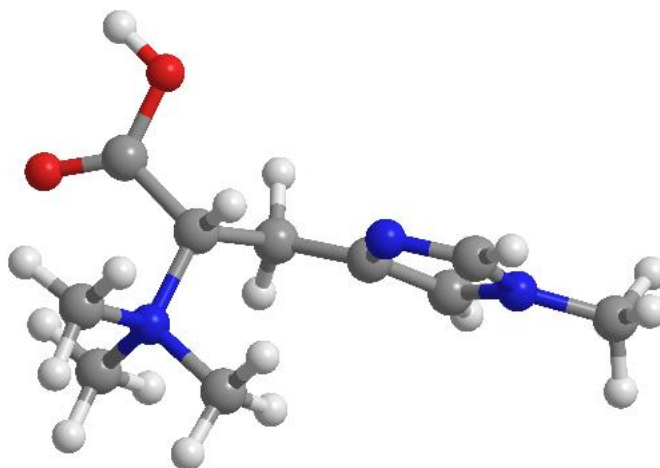
#### Kartesische Koordinaten (XYZ Format)

```
C      1.91216 -1.99268  0.36994
C      1.27434 -0.79567  0.57643
C      3.03586 -0.36838 -0.60534
N      3.02723 -1.70465 -0.38471
H      3.72491 -2.36415 -0.69499
H      1.68799 -2.99151  0.70527
N      1.99714  0.21929 -0.04076
C      0.04746 -0.57865  1.42
H      0.31321  0.07835  2.25148
H     -0.2404 -1.53192  1.86733
C     -1.17684  0.13652  0.79871
H     -1.88198  0.32613  1.60909
N     -2.00328 -0.6933 -0.21735
C     -0.70124  1.51774  0.26973
O     -0.65613  1.73055 -0.96602
O     -0.26676  2.24954  1.18066
C     -2.54045 -1.92673  0.45474
H     -1.71929 -2.58913  0.71456
H     -3.08678 -1.63846  1.35161
H     -3.20972 -2.43691 -0.2363
C     -1.21479 -1.10911 -1.43749
H     -0.80971 -0.20972 -1.88996
H     -0.41535 -1.7757 -1.12818
H     -1.8941 -1.62526 -2.11494
C     -3.17963  0.14709 -0.66488
H     -3.81061 -0.46059 -1.31173
H     -3.74095  0.45774  0.21527
H     -2.79707  1.01097 -1.19953
Na      1.41471  2.62344 -0.29773
H      3.81244  0.12143 -1.17237
```



## 5 *N*ε-Methyl-Hercynin

### 5.1 Konformer a



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

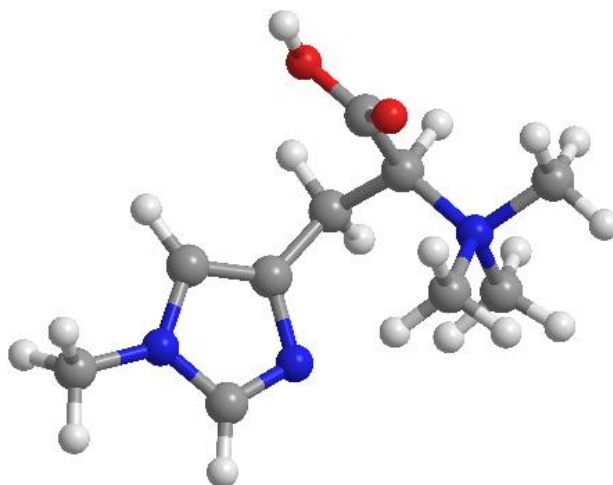
#### Kartesische Koordinaten (XYZ Format)

```
C      2.54878  0.30541 -0.98808
C      1.34991  0.36431 -0.32132
C      2.84853 -0.01084  1.16748
N      3.5025   0.06792 -0.02054
H      2.80966  0.42718 -2.02657
N      1.54847  0.16118  1.02286
C     -0.0199   0.68259 -0.86373
H     -0.17942  0.22619 -1.84341
H     -0.09318  1.76013 -1.02365
C     -1.14912  0.31247  0.12492
H     -0.71214  0.3783   1.12546
N     -1.65764 -1.13966  0.00769
C     -2.29861  1.32304  0.06669
O     -3.43942  1.10217 -0.24873
O     -1.83924  2.52058  0.44067
C     -0.48924 -2.09178  0.14263
H      0.17366 -1.97295 -0.70979
H      0.05414 -1.8579   1.05432
H     -0.88623 -3.10481  0.16809
C     -2.35288 -1.4258  -1.305
H     -3.22815 -0.79177 -1.38993
H     -1.6612  -1.23702 -2.12179
H     -2.63681 -2.47677 -1.30809
C     -2.61121 -1.43048  1.14831
H     -2.88622 -2.48253  1.10202
H     -2.09838 -1.22392  2.08633
H     -3.49492 -0.8099   1.04529
H     -2.56879  3.15977  0.39749
```



H	3.36113	-0.19665	2.09882
C	4.94121	-0.05358	-0.23869
H	5.34349	0.88038	-0.63366
H	5.42499	-0.27294	0.71195
H	5.1496	-0.86478	-0.93759

## 5.2 Konformer b



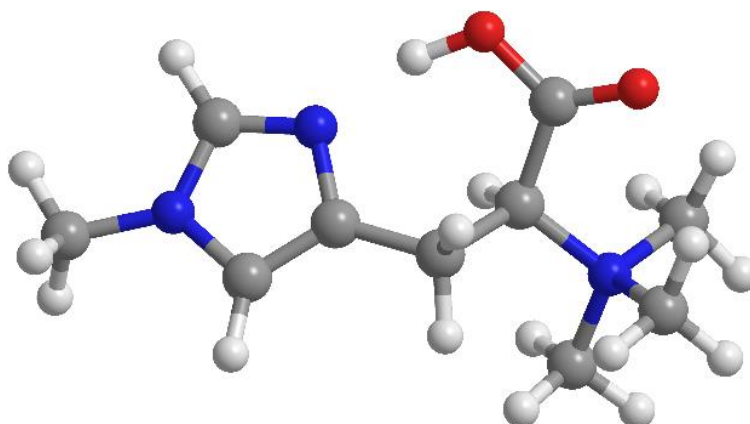
opt freq b3lyp/cc-pvtz geom=connectivity empiricdispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
C      -2.2009  0.67976 -0.46755
C      -1.14309 -0.15532 -0.7323
C      -2.60751 -1.34048  0.29863
N      -3.1327  -0.08978  0.1921
H      -2.37771  1.71591 -0.70426
N      -1.40989 -1.4179  -0.24652
C       0.11155  0.1342  -1.4919
H      -0.02174  1.04296 -2.07913
H       0.28941 -0.66321 -2.21401
C       1.4099  0.38292 -0.68359
H       2.18985  0.59204 -1.42229
N       1.97387 -0.82035  0.10827
C       1.33169  1.65189  0.18086
O       1.73881  1.77688  1.30506
O       0.78636  2.64507 -0.53109
C       1.86631 -2.0688  -0.73983
H       0.81825 -2.35161 -0.81615
H       2.2975  -1.87477 -1.72103
H       2.43017 -2.85581 -0.24271
C       1.26584 -1.10497  1.42401
H       1.39441 -0.25818  2.08678
H       0.21993 -1.30231  1.21109
H       1.73194 -1.99349  1.84724
C       3.43914 -0.568   0.3935
H       3.83239 -1.42524  0.93651
H       3.96896 -0.45852 -0.55187
H       3.5339  0.32874  0.99757
H       0.80246  3.44985  0.01196
```

H	-3.13859	-2.15021	0.77552
C	-4.44763	0.34948	0.65184
H	-4.93803	-0.47862	1.16134
H	-4.34416	1.18208	1.34887
H	-5.06113	0.65689	-0.1962

### 5.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricdispersion=gd3bj int=ultrafine pop=regular

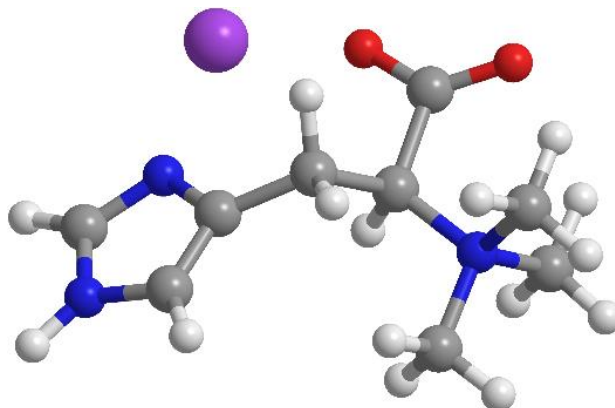
#### Kartesische Koordinaten (XYZ Format)

```
C      2.51875 -0.96494 -0.5681
C      1.39271 -0.20071 -0.40687
C      3.00273  0.85594  0.57266
N      3.53755 -0.27591  0.05801
H      2.68944 -1.90543 -1.06492
N      1.71038  0.92962  0.31144
C     -0.00785 -0.42301 -0.90404
H     -0.12477 -1.48227 -1.13012
H     -0.16673  0.11096 -1.84614
C     -1.0576  0.06002  0.13751
H     -0.62398 -0.01064  1.13687
N     -2.31125 -0.83886  0.20986
C     -1.42114  1.55327 -0.12856
O     -2.51444  1.88439 -0.52062
O     -0.44488  2.39558  0.09097
C     -1.90667 -2.21004  0.69405
H     -1.23569 -2.67951 -0.01869
H     -1.41608 -2.11482  1.66132
H     -2.80462 -2.81676  0.7933
C     -3.00545 -0.97026 -1.12818
H     -3.30556  0.01954 -1.45572
H     -2.32034 -1.42246 -1.8414
H     -3.87283 -1.61478 -0.99497
C     -3.29262 -0.28471  1.22835
H     -4.08509 -1.0182  1.36429
H     -2.76377 -0.13197  2.16823
H     -3.69431  0.6517  0.86005
H      0.44385  1.9515  0.31068
H      3.5797  1.58488  1.11939
C      4.93601 -0.69567  0.1407
H      5.36002 -0.78034 -0.86036
```

H	5.49597	0.05081	0.70148
H	5.00934	-1.65522	0.65365

## 6 *N*ε-Methyl-Hercynin+Na<sup>+</sup>

### 6.1 Konformer a



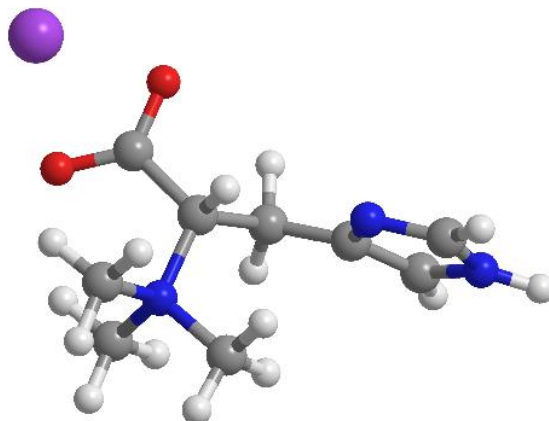
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

C	2.21642	-1.17662	-0.49472
C	1.32658	-0.1326	-0.50304
C	3.17019	0.60835	0.34979
N	3.38675	-0.69262	0.05104
H	2.13221	-2.19354	-0.8408
N	1.9422	0.98909	0.03268
C	-0.08644	-0.12978	-1.01092
H	-0.22797	-1.03334	-1.60476
H	-0.21592	0.70068	-1.70623
C	-1.17134	0.00146	0.0993
H	-0.68317	0.01706	1.0748
N	-2.10554	-1.2374	0.18698
C	-1.93846	1.37614	-0.04132
O	-3.15247	1.38519	-0.22164
O	-1.12769	2.33407	0.05079
C	-1.29321	-2.47641	0.43831
H	-0.65552	-2.6837	-0.41615
H	-0.68123	-2.32581	1.32622
H	-1.97158	-3.31437	0.5926
C	-2.927	-1.41877	-1.06763
H	-3.51807	-0.51844	-1.20678
H	-2.26036	-1.57537	-1.91253
H	-3.56087	-2.2947	-0.93596
C	-3.04608	-1.06108	1.36096
H	-3.6513	-1.96192	1.45211
H	-2.44952	-0.92241	2.2617
H	-3.66438	-0.18977	1.17178
Na	0.82419	3.07972	0.20864
H	3.93312	1.23263	0.78948

C	4.6261	-1.44172	0.24363
H	5.3667	-0.78981	0.70433
H	4.45075	-2.2964	0.89809
H	5.00787	-1.78898	-0.71726

## 6.2 Konformer b



opt freq b3lyp/cc-pvtz geom=connectivity empiricdispersion=gd3bj int=ultrafine pop=regular

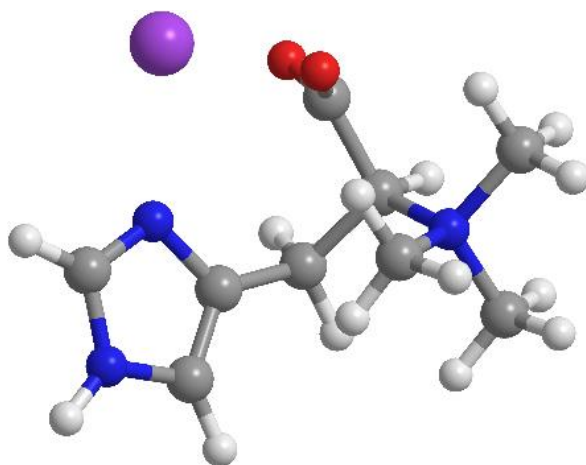
### Kartesische Koordinaten (XYZ Format)

```
C      -2.82726  0.61845  0.95595
C      -1.64486  0.44471  0.27919
C      -3.20745  0.30783 -1.18691
N      -3.8227  0.53277  0.00361
H      -3.04829  0.81095  1.993
N      -1.8964  0.24643 -1.05829
C      -0.23721  0.52675  0.80966
H      -0.17224  0.10948  1.81863
H      0.04228  1.57795  0.89663
C      0.8228  -0.07905 -0.12832
H      0.44559  0.04473 -1.14607
N      1.00315 -1.61434  0.02614
C      2.15549  0.71969 -0.06421
O      3.2629  0.127  0.07081
O      2.01605  1.95547 -0.19399
C      -0.33563 -2.30843 -0.03823
H      -0.92847 -2.03648  0.83054
H      -0.85446 -1.99099 -0.93886
H      -0.15751 -3.38274 -0.04498
C      1.6692  -1.98423  1.32748
H      2.65954 -1.54232  1.34314
H      1.06644 -1.60884  2.15106
H      1.72322 -3.07052  1.38449
C      1.8326  -2.13501 -1.12563
H      1.92192 -3.2156  -1.02327
H      1.316  -1.8935  -2.05331
H      2.80765 -1.66185 -1.08887
Na     4.24933  2.18149 -0.09892
H      -3.75801  0.19364 -2.1083
C      -5.25508  0.67629  0.23669
H      -5.48007  1.67518  0.61408
```



H	-5.78309	0.52784	-0.70432
H	-5.59878	-0.06909	0.95573

### 6.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

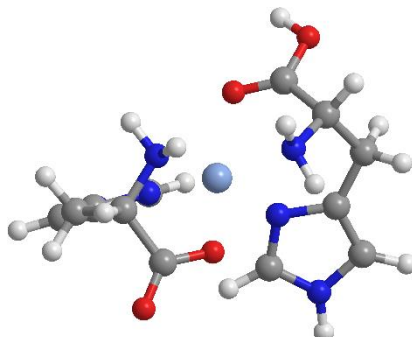
#### Kartesische Koordinaten (XYZ Format)

```
C      2.09421 -1.18618  0.61015
C      1.10505 -0.23926  0.71506
C      2.7176  0.64784 -0.41361
N      3.11631 -0.61046 -0.11254
H      2.1686  -2.18853  0.99935
N      1.51446  0.91693  0.06632
C     -0.17784 -0.37778  1.489
H     -0.18112  0.36662  2.28877
H     -0.18392 -1.35184  1.98194
C     -1.52271 -0.11018  0.77042
H     -2.30172 -0.11992  1.53401
N     -1.98245 -1.19944 -0.23307
C     -1.47081  1.32772  0.18341
O     -1.42618  1.49277 -1.05967
O     -1.33649  2.19578  1.06794
C     -2.14193 -2.51193  0.48307
H     -1.17038 -2.86835  0.81404
H     -2.80229 -2.37692  1.33847
H     -2.57523 -3.23502 -0.20628
C     -1.03061 -1.39084 -1.39108
H     -0.9053  -0.42834 -1.87644
H     -0.08109 -1.75248 -1.00795
H     -1.46916 -2.12459 -2.06651
C     -3.3345  -0.79552 -0.77955
H     -3.70042 -1.59661 -1.42007
H     -4.01774 -0.64699  0.05555
H     -3.21265  0.12443 -1.34288
Na      0.24511  2.99621 -0.35492
H      3.33987  1.32536 -0.97876
C      4.39492 -1.23038 -0.45046
```

H	4.97934	-0.53356	-1.04943
H	4.94923	-1.46878	0.45828
H	4.23059	-2.14114	-1.02767

## 7 [Ni<sup>2+</sup>(His)(His-H)]<sup>+</sup>

### 7.1 Konformer a



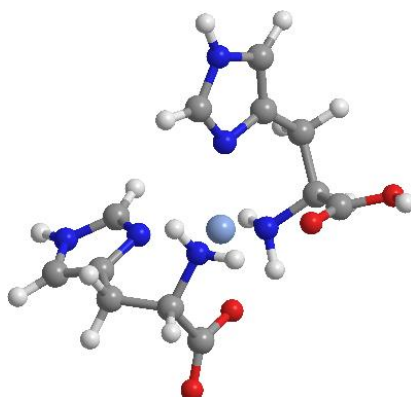
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
N      -1.41934 -1.66703 -1.31098
H      -1.09224 -1.99916 -2.21414
C      -2.56887 -0.73261 -1.53994
H      -3.17818 -1.07006 -2.38072
C      -3.47664 -0.66872 -0.3072
C      -2.04746 0.69552 -1.90094
H      -4.27366 0.0384 -0.54689
H      -3.95394 -1.64437 -0.1545
C      -2.8001 -0.24788 0.97047
O      -2.85093 1.48271 -2.35938
N      -1.42621 -0.12453 1.10906
C      -3.38313 0.04102 2.17606
C      -1.18874 0.22193 2.36317
N      -2.34983 0.33308 3.04198
H      -4.41477 0.06548 2.48246
H      -0.2149 0.39637 2.78788
O      -0.79882 0.89961 -1.6322
N      1.68337 -0.90246 -1.62491
H      1.8591 -0.09853 -2.22221
C      2.8165 -1.1616 -0.71422
H      3.56611 -1.82179 -1.15912
C      3.53819 0.13951 -0.29151
C      2.2687 -1.88315 0.5143
H      4.20993 -0.10597 0.53588
H      4.17696 0.45056 -1.1224
C      2.61835 1.27558 0.06859
O      3.21868 -2.48946 1.21128
N      1.26558 1.10841 0.31666
C      2.92182 2.60851 0.14765
C      0.76342 2.31405 0.52304
N      1.73522 3.24498 0.4448
```

H	3.84682	3.14409	0.01878
H	-0.28139	2.53303	0.65938
O	1.09274	-1.88874	0.82758
H	1.53185	-1.69845	-2.23668
H	1.60417	4.24123	0.53729
H	-2.44569	0.58693	4.01344
H	-1.72489	-2.49122	-0.79808
Ni	-0.01884	-0.40033	-0.37373
H	2.825	-2.91021	1.99274

## 7.2 Konformer b



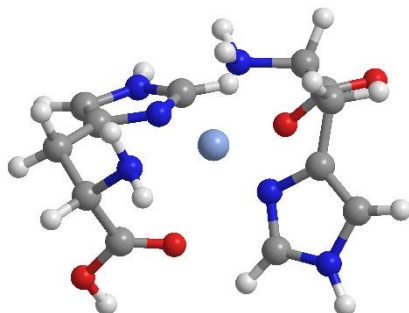
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	-1.04207	-0.64168	1.87676
H	-0.55449	-1.42194	2.31256
C	-2.39441	-1.09995	1.42756
H	-2.88002	-1.69647	2.20234
C	-3.29288	0.10547	1.12336
C	-2.2643	-1.99571	0.15613
H	-4.28301	-0.28938	0.88839
H	-3.4041	0.71301	2.03136
C	-2.84193	0.98564	-0.01173
O	-3.19978	-2.71352	-0.12975
N	-1.52797	1.07657	-0.44832
C	-3.60524	1.84413	-0.75712
C	-1.5039	1.96908	-1.4232
N	-2.7429	2.45923	-1.63951
H	-4.65968	2.05975	-0.73827
H	-0.63187	2.27545	-1.97624
O	-1.1569	-1.82521	-0.49003
N	0.94701	-0.65821	-1.7752
H	0.87839	0.00046	-2.5442
C	2.36077	-0.94548	-1.47825
H	2.86171	-1.48974	-2.28348
C	3.12824	0.37277	-1.2308
C	2.4079	-1.8048	-0.22097
H	4.19011	0.14083	-1.12612
H	3.03573	0.9723	-2.14415
C	2.68052	1.18344	-0.04142
O	3.50372	-2.54674	-0.14764
N	1.40189	1.14259	0.49763
C	3.41794	2.10903	0.64873
C	1.37291	2.02692	1.47776
N	2.5726	2.63516	1.60084
H	4.43889	2.43428	0.54269

H	0.52154	2.2441	2.10072
O	1.54866	-1.76673	0.63633
H	0.4305	-1.49742	-2.04518
H	2.80987	3.34704	2.27564
H	-2.99673	3.14384	-2.33539
H	-1.13612	0.07395	2.5934
Ni	-0.06196	-0.27656	0.06445
H	3.49481	-3.04761	0.6844

### 7.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

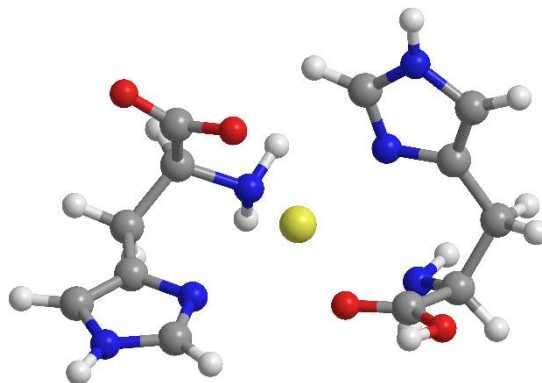
N	-1.07421	-1.32216	1.62052
H	-0.49504	-2.14374	1.7753
C	-2.32391	-1.73007	0.9042
H	-2.73067	-2.64714	1.33465
C	-3.3907	-0.63134	1.02759
C	-2.00377	-2.01539	-0.59704
H	-4.32504	-1.04874	0.64888
H	-3.55547	-0.40571	2.08981
C	-3.09746	0.63288	0.27058
O	-2.7753	-2.71936	-1.21486
N	-1.81473	1.11364	0.04506
C	-3.98914	1.48241	-0.32444
C	-1.93546	2.21814	-0.67518
N	-3.23745	2.47962	-0.90938
H	-5.06314	1.45617	-0.39004
H	-1.11791	2.79827	-1.06748
O	-0.93289	-1.43184	-1.03801
N	0.95768	1.33455	1.55332
H	1.05951	0.97358	2.49722
C	2.28878	1.67424	1.0107
H	2.71254	2.56323	1.48839
C	3.28104	0.50379	1.20776
C	2.1158	1.982	-0.47192
H	4.28701	0.87151	1.00086
H	3.26155	0.23149	2.26979
C	3.00631	-0.69111	0.3426
O	3.19699	2.55222	-0.99153
N	1.72407	-1.08417	-0.0055
C	3.90125	-1.54631	-0.24113
C	1.84021	-2.14781	-0.78565
N	3.1428	-2.46211	-0.941
H	4.97702	-1.58349	-0.21899
H	1.00582	-2.64003	-1.25995
O	1.11316	1.71454	-1.09989



H	0.37417	2.16488	1.62005
H	3.49806	-3.22779	-1.49418
H	-3.59615	3.25162	-1.4504
H	-1.30448	-0.95194	2.5398
Ni	-0.10379	-0.0742	0.20586
H	3.05775	2.68676	-1.94303

8 [Ca<sup>2+</sup>(His)(His-H)]<sup>+</sup>

### 8.1 Konformer a



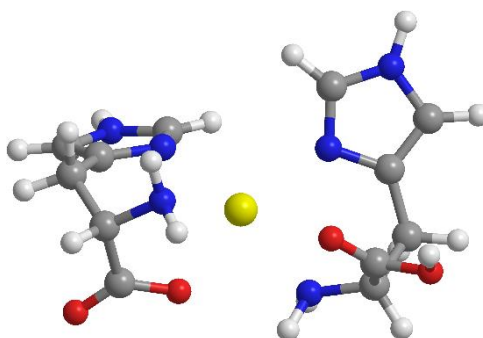
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
N      -1.07421 -1.32216  1.62052
H      -0.49504 -2.14374  1.7753
C      -2.32391 -1.73007  0.9042
H      -2.73067 -2.64714  1.33465
C      -3.3907  -0.63134  1.02759
C      -2.00377 -2.01539 -0.59704
H      -4.32504 -1.04874  0.64888
H      -3.55547 -0.40571  2.08981
C      -3.09746  0.63288  0.27058
O      -2.7753  -2.71936 -1.21486
N      -1.81473  1.11364  0.04506
C      -3.98914  1.48241 -0.32444
C      -1.93546  2.21814 -0.67518
N      -3.23745  2.47962 -0.90938
H      -5.06314  1.45617 -0.39004
H      -1.11791  2.79827 -1.06748
O      -0.93289 -1.43184 -1.03801
N       0.95768  1.33455  1.55332
H       1.05951  0.97358  2.49722
C       2.28878  1.67424  1.0107
H       2.71254  2.56323  1.48839
C       3.28104  0.50379  1.20776
C       2.1158  1.982  -0.47192
H       4.28701  0.87151  1.00086
H       3.26155  0.23149  2.26979
C       3.00631 -0.69111  0.3426
O       3.19699  2.55222 -0.99153
N       1.72407 -1.08417 -0.0055
C       3.90125 -1.54631 -0.24113
C       1.84021 -2.14781 -0.78565
```

N	3.1428	-2.46211	-0.941
H	4.97702	-1.58349	-0.21899
H	1.00582	-2.64003	-1.25995
O	1.11316	1.71454	-1.09989
H	0.37417	2.16488	1.62005
H	3.49806	-3.22779	-1.49418
H	-3.59615	3.25162	-1.4504
H	-1.30448	-0.95194	2.5398
H	3.05775	2.68676	-1.94303
Ca	-0.10379	-0.0742	0.20586

## 8.2 Konformer b



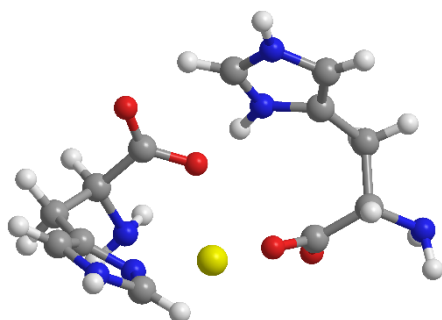
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      -1.04737 -0.65878  1.88212
H      -0.54925 -1.44829  2.2803
C     -2.39945 -1.0953   1.43423
H     -2.8855  -1.69758  2.20026
C     -3.28099  0.12418  1.16126
C     -2.28665 -1.96544  0.15391
H     -4.28679 -0.24279  0.96477
H     -3.34323  0.73082  2.07134
C     -2.85241  0.98727  0.01241
O     -3.23899 -2.65292 -0.15077
N     -1.54548  1.08394 -0.4386
C     -3.62797  1.82283 -0.74139
C     -1.53712  1.95553 -1.42928
N     -2.78089  2.42809 -1.6414
H     -4.68202  2.02794 -0.71859
H     -0.67684  2.26041 -1.99717
O     -1.17376 -1.82787 -0.4885
N      0.9391  -0.68383 -1.77428
H      0.85346 -0.05183 -2.56043
C      2.35171 -0.95024 -1.4852
H      2.85179 -1.49768 -2.28521
C      3.10082  0.37911 -1.2719
C      2.42499 -1.78671 -0.22017
H      4.1683  0.17283 -1.2126
H      2.95627  0.97127 -2.18022
C      2.68981  1.17716 -0.06873
O      3.54202 -2.49641 -0.14097
N      1.42096  1.15281  0.48973
C      3.45266  2.07448  0.62585
C      1.4223  2.01721  1.48467
N      2.63355  2.59862  1.59833
H      4.47569  2.38177  0.51064
H      0.58904  2.24051  2.12612
O      1.56968 -1.77051  0.63969
```

H	0.41414	-1.52843	-1.99437
H	2.89415	3.29212	2.2796
H	-3.04697	3.09535	-2.34564
H	-1.12649	0.03723	2.61591
H	3.5507	-2.98782	0.69617
Ca	-0.06548	-0.2736	0.06887

### 8.3 Konformer c



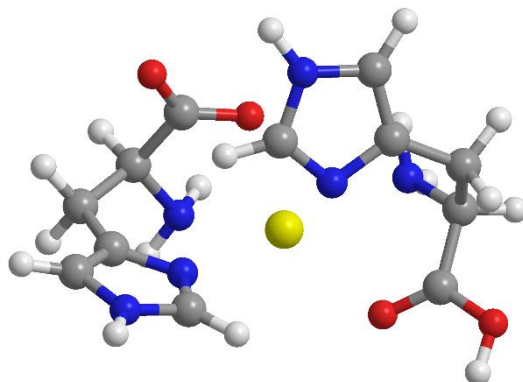
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

N	2.30585	-0.64358	2.39838
H	1.78823	-0.59841	3.27083
C	2.55995	0.74882	1.92836
H	2.87548	1.37902	2.76095
C	3.70077	0.77562	0.89299
C	1.27615	1.39668	1.36089
H	4.05259	1.80307	0.82799
H	4.53352	0.18895	1.29384
C	3.36494	0.3212	-0.4924
O	1.27189	2.58113	1.09717
N	2.59411	-0.79825	-0.78236
C	3.72484	0.91856	-1.66587
C	2.49069	-0.85635	-2.09997
N	3.16904	0.15624	-2.66959
H	4.30654	1.79867	-1.86741
H	1.91493	-1.5766	-2.65449
O	0.27499	0.57632	1.17641
N	-2.95255	-3.03499	0.97172
H	-2.25953	-3.75788	0.80181
C	-2.58592	-1.804	0.21387
H	-3.13346	-1.74569	-0.7267
C	-2.98629	-0.57779	1.08775
C	-1.07739	-1.81253	-0.18372
H	-3.89882	-0.80929	1.63456
H	-2.20257	-0.41092	1.82835
C	-3.17589	0.69451	0.33895
O	-0.72124	-0.97292	-0.99214
N	-2.10374	1.51674	0.05546
C	-4.2659	1.27174	-0.23577
C	-2.50273	2.54553	-0.67104
N	-3.81945	2.41798	-0.86223
H	-5.28775	0.94971	-0.293
H	-1.88208	3.34669	-1.02724
O	-0.35552	-2.69506	0.40931

H	-2.89372	-2.82911	1.96477
H	-4.39009	3.05967	-1.38768
H	3.24283	0.33127	-3.65761
H	3.19489	-1.07561	2.63049
H	-1.12181	1.31368	0.39513
Ca	0.74984	-1.53894	0.59944

## 8.4 Konformer d



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

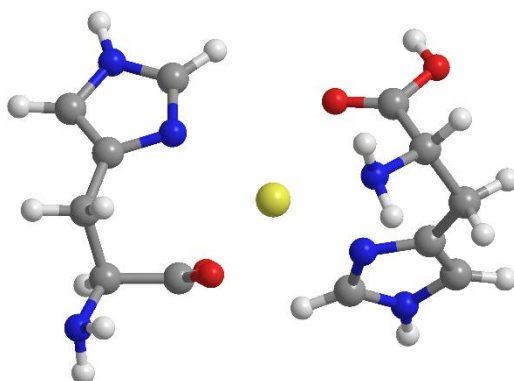
### Kartesische Koordinaten (XYZ Format)

```
N      -1.41434 -1.71415 -1.27419
H      -1.06761 -2.05584 -2.1629
C      -2.56125 -0.79304 -1.52108
H      -3.16589 -1.14842 -2.3543
C      -3.46687 -0.72048 -0.29366
C      -2.05075  0.62399 -1.90421
H      -4.29187 -0.05722 -0.54974
H      -3.90352 -1.70716 -0.11093
C      -2.80844 -0.23241  0.96279
O      -2.85998  1.40457 -2.3646
N      -1.43761 -0.11486  1.11894
C      -3.40558  0.1294  2.13842
C      -1.21586  0.29909  2.35305
N      -2.38533  0.45835  3.00224
H      -4.43931  0.18235  2.42529
H      -0.25181  0.48844  2.78825
O      -0.8001  0.84314 -1.66455
N      1.71403 -0.93038 -1.58752
H      1.8716 -0.11996 -2.17591
C      2.83167 -1.16326 -0.66183
H      3.59225 -1.81835 -1.08845
C      3.53518  0.14879 -0.25873
C      2.28713 -1.8713  0.57083
H      4.1798 -0.06631  0.59467
H      4.19955  0.43399 -1.07484
C      2.60974  1.29226  0.03489
O      3.24076 -2.46529  1.27443
N      1.25904  1.13664  0.2925
C      2.9093  2.62575  0.05482
C      0.75563  2.34696  0.45037
N      1.72546  3.2719  0.32876
H      3.8312  3.15568 -0.09793
```



H	-0.28453	2.5774	0.58834
O	1.11381	-1.88711	0.887
H	1.57767	-1.7255	-2.19938
H	1.59471	4.26847	0.38068
H	-2.49413	0.76555	3.95396
H	-1.71155	-2.52847	-0.7465
H	2.85059	-2.88118	2.05972
Ca	-0.01397	-0.42117	-0.35741

## 8.5 Konformer e



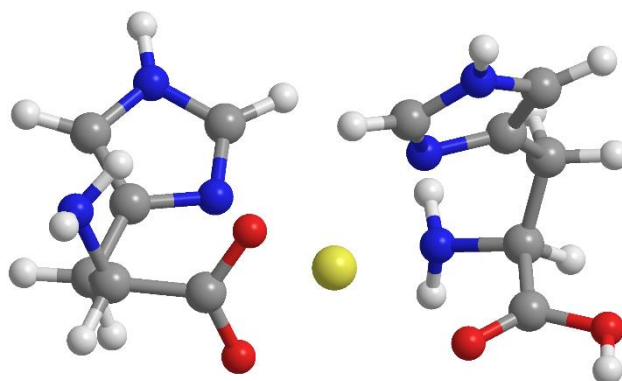
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      4.31116  1.76962 -0.24519
H      4.07626  2.72213 -0.42968
C      3.43925  0.88309 -1.04299
H      3.58957  1.12566 -2.07909
C      3.75783 -0.58933 -0.67221
C      1.97297  0.98088 -0.63889
H      4.78782 -0.79747 -0.87376
H      3.56212 -0.64675  0.37771
C      2.8792  -1.71862 -1.38198
O      1.59372  0.80427  0.63294
N      1.43273 -2.02829 -1.20314
C      3.31962 -2.662  -2.25027
C      1.21535 -3.19543 -1.7143
N      2.348  -3.57485 -2.41242
H      4.27937 -2.70863 -2.71809
H      0.28979 -3.74928 -1.61292
O      0.92133  1.10654 -1.4766
N     -1.29823 -1.19897  1.77541
H     -1.18657 -0.57099  2.55235
C     -2.75935 -1.26579  1.41341
H     -3.24242 -1.84818  2.17253
C     -3.4372  0.18259  1.40212
C     -2.94552 -1.92143 -0.01944
H     -4.49891  0.05436  1.4033
H     -3.12765  0.69253  2.2986
C     -3.11116  1.08111  0.15306
O     -3.98314 -2.63587 -0.3015
N     -1.93766  1.05332 -0.66685
C     -3.89458  2.0517  -0.40014
C     -2.05719  1.91674 -1.61607
N     -3.18064  2.59718 -1.4569
H     -4.89212  2.32587 -0.06007
```

H	-1.38236	2.08698	-2.40713
O	-2.06401	-1.73087	-0.93177
H	-0.92051	-2.09492	2.03357
H	-3.4117	3.38379	-2.04428
H	2.46496	-4.39996	-2.96648
H	4.18721	1.57839	0.73073
Ca	-0.15743	-0.49049	-0.1938
H	-4.0817	-2.98834	-1.20466

## 8.6 Konformer f



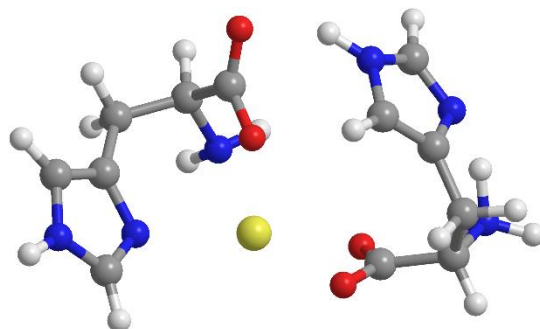
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      -2.57508  3.12427  0.33564
H      -2.05132  3.80227  0.85139
C      -2.7677  1.92287  1.16052
H      -3.30455  2.12961  2.06271
C      -4.00009  0.87704  0.204
C      -0.99604  1.53671  1.75022
H      -4.25022  0.07534  0.86702
H      -4.88675  1.41106 -0.06724
C      -3.3241  0.23762 -1.04689
O       0.13595  2.14362  1.15748
N      -2.62838  0.94213 -2.26678
C      -3.33946 -1.19905 -1.53251
C      -1.9682  0.07397 -3.24174
N      -2.34729 -1.294  -2.7264
H      -3.57492 -2.01588 -0.88269
H      -1.74733  0.28614 -4.26697
O      -0.57187  0.31706  2.30442
N       1.18171 -1.96088 -0.36791
H       1.04095 -2.29521 -1.29979
C       2.61724 -1.91003 -0.1515
H       2.99984 -2.9089  -0.12374
C       3.44649 -1.18759 -1.22704
C       2.71424 -1.23169  1.13691
H       4.48496 -1.32197 -1.00698
H       3.21939 -1.6143  -2.18163
C       3.17879  0.29814 -1.24566
O       3.69655 -1.42258  1.96877
N       1.98342  0.99529 -0.87432
C       4.06537  1.23816 -1.62477
C       2.22056  2.26135 -1.04852
N       3.47575  2.43167 -1.50267
H       5.06477  1.06115 -1.96355
H       1.52241  3.04982 -0.85932
```

O	1.75824	-0.46282	1.37445
H	0.81133	-2.60463	0.30172
H	3.90028	3.31179	-1.71517
H	-1.80985	-2.10648	-2.9523
H	-2.07692	2.88086	-0.49658
Ca	-0.13972	0.13221	-0.07238
H	3.71213	-0.9569	2.80811

## 8.7 Konformer g



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

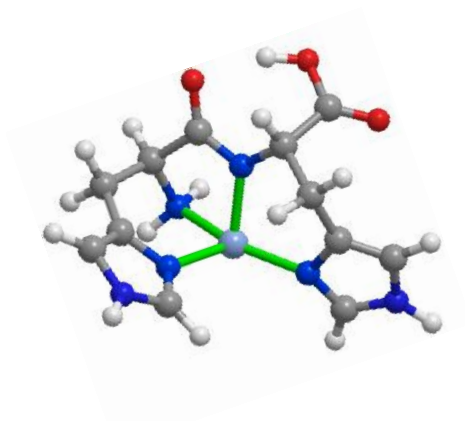
### Kartesische Koordinaten (XYZ Format)

```
N      -0.87334  1.53605 -1.5878
H      -0.19175  2.26523 -1.6489
C      -2.03037  2.00542 -0.77988
H      -2.29181  3.03237 -1.03375
C      -3.25422  1.12723 -1.06027
C      -1.70001  1.9759  0.73309
H      -4.11331  1.59932 -0.58796
H      -3.44852  1.12884 -2.13746
C      -3.13529 -0.27696 -0.55358
O      -2.46487  2.51183  1.50876
N      -1.91963 -0.90556 -0.34578
C      -4.13518 -1.13872 -0.19835
C      -2.17965 -2.11114  0.12717
N      -3.51256 -2.29218  0.22205
H      -5.20386 -1.03023 -0.19817
H      -1.44619 -2.83282  0.438
O      -0.61758  1.32955  1.04642
N      0.87346 -1.53631 -1.58773
H      1.17534 -1.31026 -2.52927
C      2.03055 -2.00544 -0.77975
H      2.29211 -3.0324  -1.03349
C      3.2543  -1.12716 -1.06024
C      1.70017 -1.97575  0.7332
H      4.11344 -1.59912 -0.58789
H      3.4486  -1.12882 -2.13743
C      3.13521  0.27705 -0.55362
O      2.46537 -2.51097  1.50903
N      1.91947  0.90539 -0.34555
C      4.135  1.13905 -0.19868
C      2.17933  2.11105  0.12727
N      3.51222  2.29238  0.22182
H      5.2037  1.03079 -0.19875
H      1.4458  2.83261  0.43821
O      0.6173  -1.33004  1.04635
```

H	0.18397	-2.27367	-1.67748
H	3.97114	3.12323	0.55582
H	-3.97158	-3.12291	0.55618
H	-1.1849	1.29316	-2.50646
H	-0.46538	0.73416	-1.15129
Ca	-0.00008	-0.00016	-0.4069

9 [Ni<sup>2+</sup>(HisHis-H)]<sup>+</sup>

9.1 a Im[NNNN]<sub>OH</sub>



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

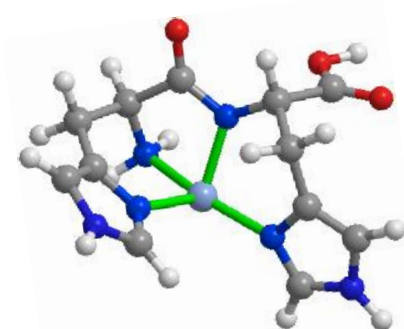
**Kartesische Koordinaten (XYZ Format)**

N	-1.39679	-0.65372	2.12408
C	-1.90349	-1.63951	1.11116
H	-2.22827	-2.56059	1.59832
C	-3.11447	-1.04936	0.36604
C	-0.75521	-2.01563	0.1519
H	-3.44231	-1.79817	-0.35834
H	-3.93522	-0.93987	1.08551
C	-2.91239	0.26629	-0.34511
O	-0.74966	-3.13103	-0.38177
N	-1.89433	1.17115	-0.0611
C	-3.69501	0.80609	-1.32886
C	-2.06016	2.21707	-0.85735
N	-3.14437	2.03365	-1.63335
H	-4.5732	0.43156	-1.8263
H	-1.41844	3.08109	-0.89891
N	0.13169	-1.03229	-0.02707
C	1.13222	-1.18885	-1.08495
H	0.67517	-1.74438	-1.91405
C	1.57006	0.18305	-1.62251
C	2.32649	-2.02483	-0.58528
H	2.32619	0.03006	-2.39257
H	0.69767	0.64088	-2.10004
C	2.1122	1.13473	-0.60412
O	2.0218	-3.28226	-0.25282
N	1.32613	1.63388	0.43372
C	3.35511	1.68711	-0.50091
C	2.09014	2.46371	1.1398
N	3.3192	2.52069	0.59737



H	4.24633	1.53187	-1.08256
H	1.7916	3.01433	2.01645
O	3.44236	-1.58316	-0.49364
H	-2.1768	-0.2579	2.64611
H	4.08861	3.07434	0.94455
H	-3.49304	2.68423	-2.32203
Ni	-0.27804	0.5945	0.93431
H	1.06866	-3.46414	-0.4082
H	-0.82144	-1.15047	2.80271

## 9.2 b Im[NNNN]



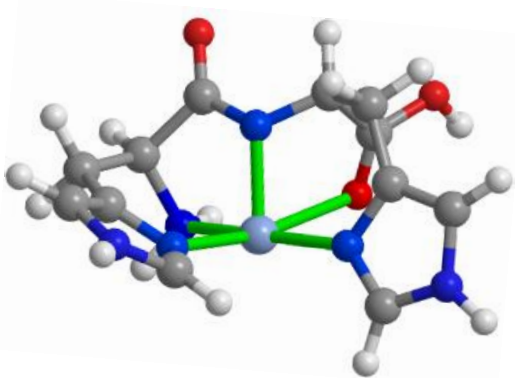
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      -1.47297 -1.02783  1.99119
C      -1.99698 -1.80117  0.81469
H      -2.34328 -2.78769  1.12913
C      -3.18978 -1.06637  0.18289
C      -0.87036 -2.03235 -0.22388
H      -3.53372 -1.68655 -0.64717
H      -4.00986 -1.03214  0.91036
C      -2.92114  0.32638 -0.32717
O      -1.04706 -2.86521 -1.10017
N      -1.84477  1.11158  0.072
C      -3.6644  1.04889 -1.21999
C      -1.93844  2.26726 -0.56954
N      -3.03191  2.26758 -1.35453
H      -4.56217  0.80474 -1.7614
H      -1.23903  3.08271 -0.49592
N      0.18334 -1.205  -0.04342
C      1.2445  -1.22874 -1.0352
H      0.93923 -1.89423 -1.85321
C      1.49348  0.17851 -1.61873
C      2.54869 -1.81118 -0.49249
H      2.23019  0.11156 -2.4188
H      0.55124  0.52305 -2.05433
C      1.9784  1.1743  -0.61113
O      2.34044 -2.83397  0.35508
N      1.25702  1.48837  0.54045
C      3.13477  1.89997 -0.59888
C      1.96972  2.38133  1.21872
N      3.10844  2.6552  0.55542
H      3.96385  1.91767 -1.2841
H      1.69916  2.82817  2.16115
O      3.6457  -1.42068 -0.80806
H      -2.24525 -0.70713  2.57226
```

H	3.82637	3.29557	0.86074
H	-3.3336	3.02866	-1.94484
Ni	-0.28132	0.33116	1.02341
H	-0.91462	-1.65453	2.56796
H	3.21106	-3.19375	0.58447

### 9.3 c Im[NNNNO]



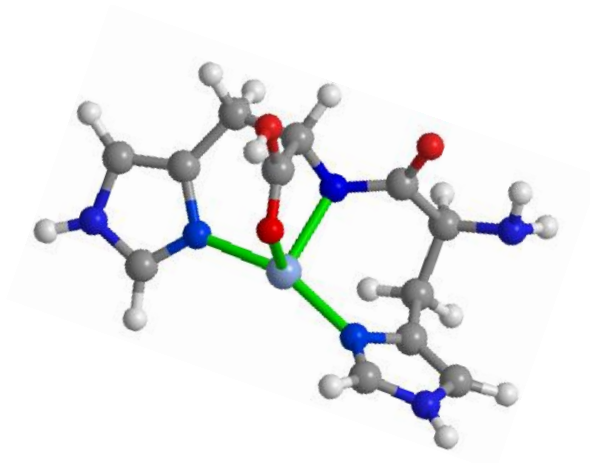
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
N      1.4253 -1.3468 -1.67008
C      2.10732 -1.83428 -0.41891
H      2.57016 -2.80725 -0.59307
C      3.22253 -0.8586 -0.01473
C      1.00673 -2.07927 0.65347
H      3.68459 -1.25106 0.89418
H      3.99953 -0.89685 -0.7892
C      2.84655 0.58193 0.21347
O      1.03188 -3.08912 1.34058
N      1.71971 1.19963 -0.31578
C      3.5552 1.51487 0.92034
C      1.75098 2.46463 0.07201
N      2.85055 2.69596 0.81542
H      4.47418 1.4413 1.47604
H      1.00052 3.20632 -0.14157
N      0.08081 -1.09635 0.64339
C      -1.2568 -1.37175 1.10073
H      -1.28333 -2.20011 1.81303
C      -1.88253 -0.10931 1.74679
C      -2.06699 -1.74708 -0.14564
H      -2.81628 -0.37101 2.24883
H      -1.17329 0.2194 2.51128
C      -2.16201 1.01656 0.78616
O      -3.18151 -2.42033 0.10538
N      -1.37063 1.319 -0.32039
C      -3.20042 1.90749 0.82175
C      -1.92374 2.36089 -0.92193
N      -3.03021 2.74965 -0.25651
H      -4.02342 2.01109 1.50785
H      -1.57142 2.83044 -1.8259
O      -1.72611 -1.41156 -1.27123
H      2.11893 -1.07376 -2.36369
```

H	-3.63699	3.51335	-0.51509
H	3.11128	3.57961	1.22647
Ni	0.12819	0.07681	-0.89966
H	0.89279	-2.11358	-2.07747
H	-3.64036	-2.5945	-0.73261

## 9.4 d Im[NNNO]



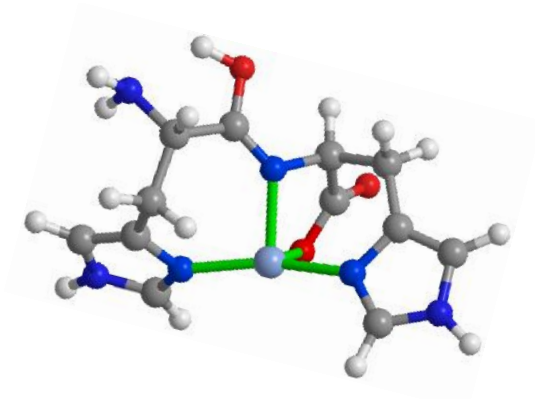
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      3.43474  1.81205 -1.19439
H      3.96277  2.04103 -2.0291
C      2.10879  1.31483 -1.54516
H      1.72365  1.74928 -2.48224
C      2.18741 -0.21347 -1.77939
C      1.09045  1.8051  -0.48791
H      1.23165 -0.58316 -2.16836
H      2.92204 -0.39175 -2.56742
C      2.57315 -0.96721 -0.55187
O      1.28796  2.89937  0.03516
N      1.59972 -1.43452  0.32262
C      3.79576 -1.21406  0.00139
C      2.22002 -1.95301  1.375
N      3.55073 -1.8407  1.20785
H      4.78623 -0.96761 -0.33523
H      1.74752 -2.38711  2.23976
N      -0.0249  1.04798 -0.29839
C      -1.04377  1.64392  0.55911
H      -0.78534  2.67435  0.81132
C      -2.42125  1.63263 -0.14647
C      -1.12185  0.85006  1.85187
H      -3.16991  2.11836  0.48543
H      -2.2992  2.25116 -1.03938
C      -2.92509  0.27191 -0.55417
O      -0.77984 -0.33422  1.91511
N      -2.13529 -0.87357 -0.60731
C      -4.18671 -0.06593 -0.96152
C      -2.9054  -1.86332 -1.04026
N      -4.15132 -1.40994 -1.26705
H      -5.0816  0.52337 -1.06433
```

H	-2.60045	-2.88599	-1.18928
O	-1.61575	1.49285	2.88756
H	3.32099	2.6681	-0.65801
H	-4.92601	-1.96252	-1.60365
H	4.2511	-2.15933	1.86077
Ni	-0.23982	-0.87884	-0.00302
H	-1.65222	0.89736	3.65466

## 9.5 e II[NNNO]<sub>OH</sub>



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

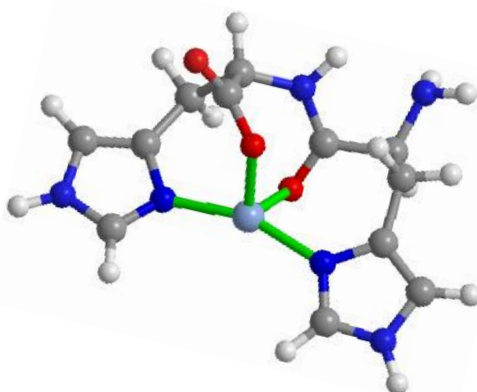
### Kartesische Koordinaten (XYZ Format)

```
N      3.51072  1.96308 -1.01315
H      3.53384  2.9628  -1.00834
C      2.16316  1.50587 -1.38184
H      1.88321  1.85711 -2.35301
C      2.22989 -0.1136  -1.54775
C      1.10568  2.23851 -0.3801
H      1.21717 -0.42817 -1.69039
H      2.81754 -0.27697 -2.42689
C      2.88251 -1.11722 -0.46469
O      1.3293  3.45352 -0.14071
N      2.17514 -1.76574  0.59537
C      4.14268 -1.59889 -0.36967
C      2.91981 -2.68857  1.16715
N      4.15329 -2.57315  0.59837
H      4.98128 -1.28615 -0.95605
H      2.62252 -3.37697  1.93045
N      -0.00045  1.70661  0.21843
C      -1.41826  2.15552  0.75492
H      -1.38988  3.22213  0.83515
C      -2.61748  1.71634 -0.3594
C      -1.80535  1.55704  2.32902
H      -3.51487  2.19659 -0.02932
H      -2.27603  2.121  -1.28921
C      -3.08894  0.1187  -0.69929
O      -1.42514  0.3767  2.91789
N      -2.42825 -1.19423 -0.50577
C      -4.25784 -0.26303 -1.28543
C      -3.09725 -2.18388 -1.03731
N      -4.24537 -1.62554 -1.50587
H      -5.06043  0.39536 -1.54478
H      -2.80826 -3.21303 -1.08453
O      -2.55297  2.33382  3.05777
```



H	3.74166	1.61994	-0.10269
H	-4.98254	-2.13438	-1.95047
H	4.95193	-3.11979	0.85007
Ni	-0.25491	-0.6809	0.87309
H	4.17338	1.61752	-1.67758

## 9.6 f CS[NNOO]



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

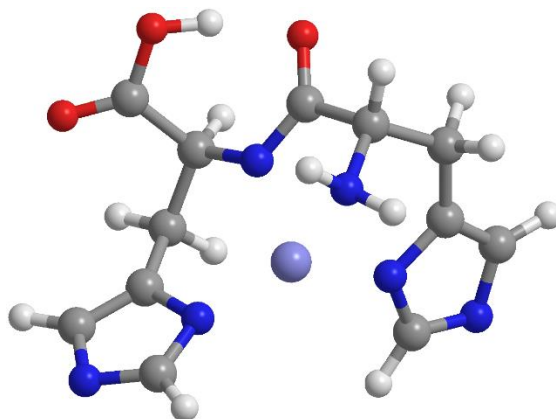
### Kartesische Koordinaten (XYZ Format)

```
N      2.44091  3.22474 -0.49753
H      3.34287  3.4056  -0.07287
C      2.24066  1.80725 -0.78525
H      2.70688  1.45115 -1.71073
C      2.77705  0.96869  0.41952
C      0.75354  1.4925  -0.86463
H      3.77661  1.34344  0.65468
H      2.14104  1.1663  1.28733
C      2.89551 -0.51239  0.22791
O      0.38718  0.4138  -1.40212
N      1.82329 -1.40196  0.20876
C      4.05083 -1.23981  0.1404
C      2.33251 -2.62072  0.10955
N      3.67698 -2.56316  0.06491
H      5.08267 -0.93327  0.14447
H      1.77179 -3.54013  0.07041
N      -0.05474  2.32033 -0.22271
H      0.43618  3.11488  0.1847
C      -1.39822  2.00394  0.27512
H      -1.81579  2.94585  0.62237
C      -2.34452  1.42923 -0.83129
C      -1.32826  1.09007  1.55435
H      -3.2183  2.07734 -0.90257
H      -1.8324  1.47925 -1.79281
C      -2.84596  0.03319 -0.62063
O      -2.13532  1.29215  2.43101
N      -2.02384 -1.07496 -0.43631
C      -4.14383 -0.39265 -0.59201
C      -2.8149  -2.12971 -0.29807
N      -4.10362 -1.7558  -0.39484
H      -5.0688  0.14889 -0.68756
```

H	-2.49575	-3.14356	-0.12232
O	-0.39767	0.17585	1.54039
H	2.37931	3.78607	-1.34045
Ni	-0.09989	-0.90906	-0.00142
H	-4.90147	-2.36905	-0.32016
H	4.29932	-3.35538	0.00527

10 [Ni<sup>2+</sup>(HisHis-3H)]<sup>-</sup>

10.1 a Im[NNNN]<sub>OH</sub>



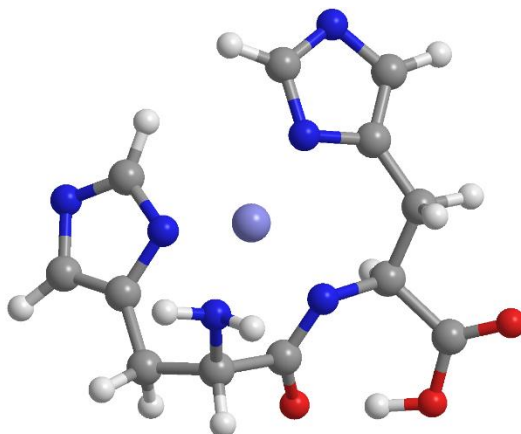
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

N	1.36457	-0.91998	-1.94126
C	1.83391	-1.84096	-0.86734
H	2.07434	-2.82216	-1.28181
C	3.10911	-1.28025	-0.22843
C	0.68802	-2.08455	0.1382
H	3.39102	-1.97368	0.5655
H	3.90532	-1.34844	-0.98297
C	3.04069	0.11811	0.31942
O	0.69319	-3.13035	0.79796
N	2.04046	1.01965	0.02531
C	3.92681	0.76715	1.15168
C	2.37146	2.14717	0.70576
N	3.50337	2.05167	1.38975
H	4.83335	0.37922	1.59194
H	1.74205	3.02326	0.68544
N	-0.19744	-1.09329	0.15464
C	-1.36089	-1.19279	0.9875
H	-1.1864	-1.90888	1.79654
C	-1.71494	0.18168	1.607
C	-2.54185	-1.73172	0.1929
H	-2.54499	0.05584	2.30063
H	-0.83966	0.48341	2.18808
C	-2.07182	1.23841	0.61261
O	-3.63763	-1.89861	0.98497
N	-1.21705	1.61758	-0.40366
C	-3.19551	2.0248	0.50136
C	-1.87799	2.60781	-1.06174
N	-3.06922	2.89228	-0.55878
H	-4.07544	2.01659	1.12628

H	-1.45066	3.1065	-1.91917
O	-2.56927	-2.00144	-0.97946
H	2.14369	-0.60908	-2.51044
Ni	0.34081	0.52632	-0.81639
H	0.70125	-1.39921	-2.53918
H	1.59962	-3.3978	0.96667

## 10.2 b Im[NNNN]<sub>OH</sub>



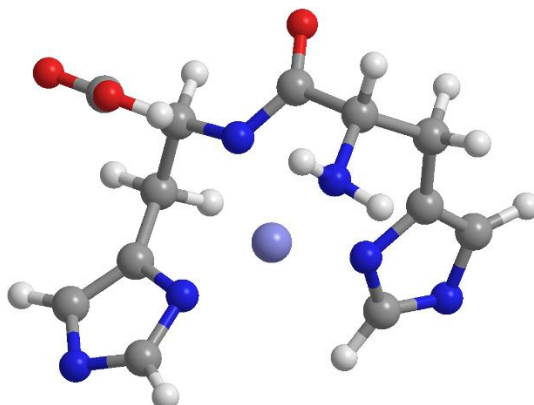
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

```
N      1.55373  0.72079  2.33112
C      1.69593  1.80604  1.2684
H      2.06913  2.70273  1.71735
C      2.85618  1.18881  0.26733
C      0.21008  2.23513  0.51388
H      3.04728  1.91557 -0.49438
H      3.70697  1.06334  0.90397
C      2.67591 -0.2726  -0.50787
O      0.01407  3.43186  0.17775
N      1.78245 -1.29572 -0.38062
C      3.50937 -0.70627 -1.4903
C      2.11909 -2.33815 -1.11408
N      3.19852 -1.98629 -1.84381
H      4.30306 -0.12968 -1.91749
H      1.62077 -3.28477 -1.13619
N      -0.76384  1.3081  0.28001
C      -2.17295  1.21502 -0.09514
H      -2.23491  1.02748 -1.14676
C      -2.91039  0.01788  0.72818
C      -2.88549  2.53899  0.23802
H      -2.89648  0.29356  1.76197
H      -3.9128  -0.01678  0.35554
C      -2.32628 -1.51118  0.66309
O      -4.10941  2.53855  0.53054
N      -0.95576 -2.06516  0.63658
C      -3.08512 -2.63049  0.64652
C      -1.02311 -3.38405  0.60378
N      -2.29127 -3.74792  0.60939
H      -4.15496 -2.64245  0.66084
H      -0.18534 -4.04912  0.57674
O      -2.22193  3.6582  0.21704
```

H	2.42217	0.40769	2.71553
Ni	0.40831	-0.90838	0.63699
H	0.96509	0.97052	3.09997
H	-1.28823	3.65854	-0.00612

### 10.3 c Im[NNNN]



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

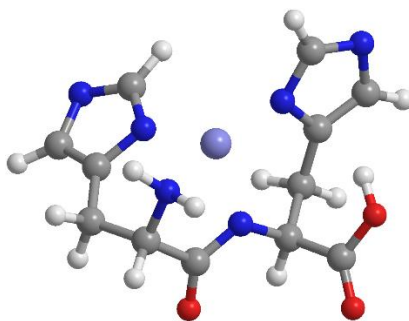
#### Kartesische Koordinaten (XYZ Format)

```
N      1.30427  0.46861  2.08275
C      1.72581  1.59283  1.20484
H      1.91404  2.493    1.79306
C      3.02867  1.22105  0.48665
C      0.58464  1.94664  0.24196
H      3.28635  2.06126 -0.15971
H      3.81411  1.1809   1.25394
C      3.01766 -0.05154 -0.31213
O      0.5404   3.12391 -0.19679
N      2.06545 -1.04025 -0.18058
C      3.92102 -0.49199 -1.25442
C      2.44177 -2.00687 -1.05769
N      3.55635 -1.73088 -1.71967
H      4.80151  0.01397 -1.62114
H      1.85865 -2.90457 -1.19303
N      -0.25318  0.9645  -0.01086
C      -1.30625  1.14869 -1.00812
H      -0.87633  1.70326 -1.8533
C      -1.80642 -0.20112 -1.5455
C      -2.45588  2.04447 -0.51057
H      -2.65944 -0.00471 -2.19262
H      -1.00469 -0.60305 -2.1726
C      -2.19808 -1.23387 -0.53909
O      -3.24841  2.59022 -1.23591
N      -1.28032 -1.77121  0.34544
C      -3.37934 -1.90388 -0.33807
C      -1.97125 -2.72986  1.02724
N      -3.23242 -2.84967  0.6537
H      -4.32031 -1.75137 -0.84163
H      -1.50853 -3.32546  1.8005
O      -2.48034  2.23121  0.8157
H      2.10596  0.07142  2.55895
```



Ni	0.33856	-0.79415	0.71447
H	0.64973	0.79594	2.78349
H	-1.70963	1.75704	1.24001

## 10.4 d Im[NNNN]

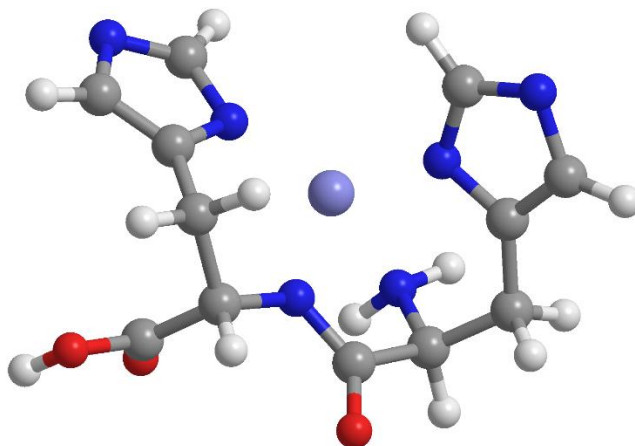


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	1.45049	-1.08388	-1.87812
C	1.89116	-1.88803	-0.7038
H	2.17972	-2.8976	-1.01324
C	3.13689	-1.24051	-0.05754
C	0.71145	-2.06689	0.26557
H	3.38581	-1.85851	0.8062
H	3.96565	-1.37043	-0.76823
C	3.02428	0.19417	0.3511
O	0.75943	-3.02587	1.06673
N	2.01886	1.01278	-0.09059
C	3.8229	0.95367	1.1868
C	2.23589	2.20121	0.52134
N	3.32378	2.22338	1.28841
H	4.72185	0.6528	1.70416
H	1.57178	3.03862	0.3763
N	-0.24807	-1.14198	0.13649
C	-1.43383	-1.21086	0.95157
H	-1.23942	-1.9101	1.77175
C	-1.74201	0.16713	1.55795
C	-2.61049	-1.85452	0.18789
H	-2.61019	0.05661	2.22137
H	-0.89304	0.40378	2.20333
C	-2.00352	1.2862	0.59358
O	-2.50842	-2.62164	-0.73206
N	-1.20347	1.55828	-0.50591
C	-3.00499	2.23592	0.59244
C	-1.80193	2.60397	-1.11933
N	-2.87961	3.06003	-0.49119
H	-3.78374	2.38408	1.32587
H	-1.40622	3.03844	-2.02265
O	-3.84993	-1.52284	0.59251
H	2.2544	-0.85092	-2.43565
Ni	0.32363	0.40485	-0.90813
H	0.82211	-1.63098	-2.44748
H	-3.82741	-0.7177	1.10924

10.5 e Im[NNNN]



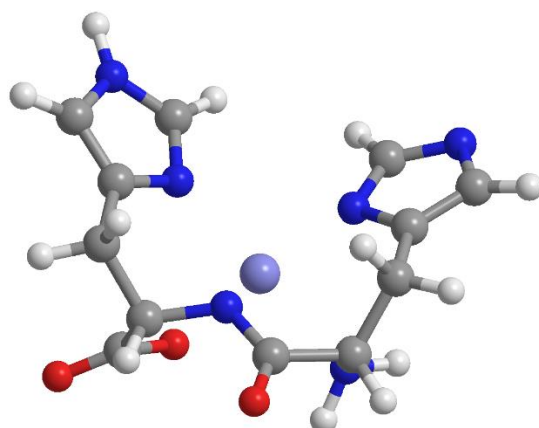
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

**Kartesische Koordinaten (XYZ Format)**

N	1.42955	-1.31991	-1.68237
C	2.1081	-1.8159	-0.4419
H	2.56869	-2.78518	-0.62326
C	3.22063	-0.84784	-0.03285
C	1.01057	-2.06084	0.62076
H	3.69391	-1.25205	0.86167
H	3.98756	-0.87396	-0.81414
C	2.84522	0.58218	0.22294
O	1.01088	-3.0924	1.27541
N	1.72816	1.21188	-0.30682
C	3.54398	1.50092	0.95304
C	1.75425	2.46818	0.10025
N	2.84375	2.68303	0.85913
H	4.45444	1.41756	1.51682
H	1.01273	3.21627	-0.11189
N	0.10766	-1.06055	0.65606
C	-1.22233	-1.34298	1.12173
H	-1.23182	-2.15187	1.85239
C	-1.86144	-0.08435	1.74749
C	-2.03702	-1.76586	-0.09933
H	-2.78362	-0.35318	2.26052
H	-1.15715	0.26727	2.50291
C	-2.16895	1.01523	0.77498
O	-3.14163	-2.44095	0.18857
N	-1.39045	1.31533	-0.33808
C	-3.2234	1.88349	0.79714
C	-1.96433	2.33199	-0.9575
N	-3.07373	2.70794	-0.29505
H	-4.04519	1.98257	1.48169
H	-1.62596	2.79367	-1.86815
O	-1.7151	-1.47297	-1.23984

H	2.11458	-1.03631	-2.37592
Ni	0.12687	0.09255	-0.91283
H	0.88395	-2.07069	-2.09427
H	-3.60835	-2.65293	-0.63574

## 10.6 f Im[NNNN]



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

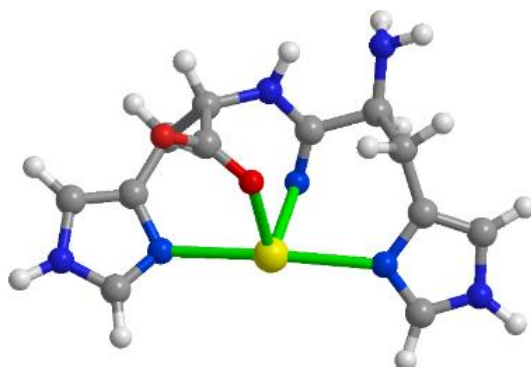
### Kartesische Koordinaten (XYZ Format)

```
N      1.42955 -1.31991 -1.68237
C      2.1081  -1.8159  -0.4419
H      2.56869 -2.78518 -0.62326
C      3.22063 -0.84784 -0.03285
C      1.01057 -2.06084  0.62076
H      3.69391 -1.25205  0.86167
H      3.98756 -0.87396 -0.81414
C      2.84522  0.58218  0.22294
O      1.01088 -3.0924  1.27541
N      1.72816  1.21188 -0.30682
C      3.54398  1.50092  0.95304
C      1.75425  2.46818  0.10025
N      2.84375  2.68303  0.85913
H      4.45444  1.41756  1.51682
H      1.01273  3.21627 -0.11189
N      0.10766 -1.06055  0.65606
C      -1.22233 -1.34298  1.12173
H      -1.23182 -2.15187  1.85239
C      -1.86144 -0.08435  1.74749
C      -2.03702 -1.76586 -0.09933
H      -2.78362 -0.35318  2.26052
H      -1.15715  0.26727  2.50291
C      -2.16895  1.01523  0.77498
O      -3.14163 -2.44095  0.18857
N      -1.39045  1.31533 -0.33808
C      -3.2234  1.88349  0.79714
C      -1.96433  2.33199 -0.9575
N      -3.07373  2.70794 -0.29505
H      -4.04519  1.98257  1.48169
H      -1.62596  2.79367 -1.86815
O      -1.7151  -1.47297 -1.23984
```

H	2.11458	-1.03631	-2.37592
Ni	0.12687	0.09255	-0.91283
H	0.88395	-2.07069	-2.09427
H	-3.68422	3.45715	-0.55193

11 [Ca<sup>2+</sup>(HisHis-H)]<sup>+</sup>

11.1 a CS[NNOO]



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

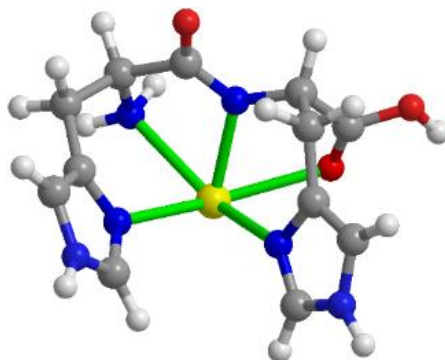
**Kartesische Koordinaten (XYZ Format)**

N	2.37418	3.4373	-0.56065
H	3.35677	3.58598	-0.67209
C	2.05888	2.02629	-0.82624
H	2.35036	1.77091	-1.82359
C	2.90761	1.07648	0.23892
C	0.48649	1.86638	-0.63448
H	3.91725	1.43077	0.24037
H	2.43638	1.24641	1.18442
C	3.0552	-0.579	0.04327
O	0.02381	0.88957	-1.25441
N	2.0637	-1.65554	0.26546
C	4.1549	-1.28014	-0.33138
C	2.61212	-2.84346	0.21563
N	3.89874	-2.62935	-0.18552
H	5.07708	-0.8558	-0.66965
H	2.14613	-3.78311	0.4273
N	-0.38205	2.69036	0.25521
H	-0.08362	3.58856	0.57796
C	-1.72617	2.07678	0.73077
H	-2.50303	2.68854	1.13961
C	-2.18203	1.32254	-0.60794
C	-1.14165	1.11851	1.6937
H	-2.71363	2.02041	-1.22054
H	-1.26973	1.02041	-1.07839
C	-2.99748	-0.02232	-0.50117
O	0.10512	1.33599	1.69272
N	-2.25439	-1.21309	-0.19979
C	-4.27693	-0.39975	-0.65334
C	-3.03489	-2.26832	-0.3281
N	-4.29494	-1.77711	-0.58113
H	-5.1177	0.24246	-0.81326
H	-2.74961	-3.29575	-0.23914

O	-1.53823	-0.12953	2.24346
H	1.87423	4.01734	-1.20377
H	-5.11234	-2.34155	-0.69631
H	4.56745	-3.35379	-0.3529
Ca	-0.02019	-0.65055	0.48446



## 11.2 b Im[NNNNO]



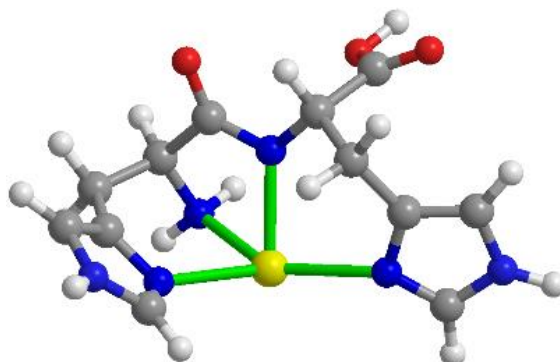
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	1.4253	-1.3468	-1.67008
C	2.10732	-1.83428	-0.41891
H	2.57016	-2.80725	-0.59307
C	3.22253	-0.8586	-0.01473
C	1.00673	-2.07927	0.65347
H	3.68459	-1.25106	0.89418
H	3.99953	-0.89685	-0.7892
C	2.84655	0.58193	0.21347
O	1.03188	-3.08912	1.34058
N	1.71971	1.19963	-0.31578
C	3.5552	1.51487	0.92034
C	1.75098	2.46463	0.07201
N	2.85055	2.69596	0.81542
H	4.47418	1.4413	1.47604
H	1.00052	3.20632	-0.14157
N	0.08081	-1.09635	0.64339
C	-1.2568	-1.37175	1.10073
H	-1.28333	-2.20011	1.81303
C	-1.88253	-0.10931	1.74679
C	-2.06699	-1.74708	-0.14564
H	-2.81628	-0.37101	2.24883
H	-1.17329	0.2194	2.51128
C	-2.16201	1.01656	0.78616
O	-3.18151	-2.42033	0.10538
N	-1.37063	1.319	-0.32039
C	-3.20042	1.90749	0.82175
C	-1.92374	2.36089	-0.92193
N	-3.03021	2.74965	-0.25651
H	-4.02342	2.01109	1.50785
H	-1.57142	2.83044	-1.8259
O	-1.72611	-1.41156	-1.27123
H	2.11893	-1.07376	-2.36369
H	-3.63699	3.51335	-0.51509

H	3.11128	3.57961	1.22647
H	0.89279	-2.11358	-2.07747
H	-3.64036	-2.5945	-0.73261
Ca	0.14044	0.37996	-1.2984

### 11.3 c Im[NNNN]



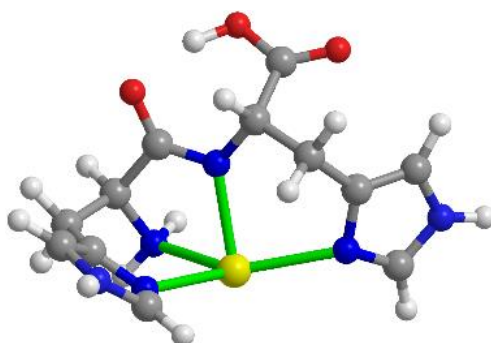
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
N      1.50899  1.02618  1.99317
C      2.055   1.75448  0.80696
H      2.42775  2.73494  1.09976
C      3.22342  0.96882  0.20405
C      0.94545  1.98228 -0.23907
H      3.63155  1.57419 -0.60355
H      4.01303  0.88148  0.95664
C      2.89   -0.392  -0.33342
O      1.14543  2.78018 -1.14244
N      1.80032 -1.14693  0.08013
C      3.57322 -1.11758 -1.26671
C      1.82778 -2.28752 -0.58885
N      2.89273 -2.3066  -1.40825
H      4.45925 -0.89354 -1.83103
H      1.10584 -3.08011 -0.51274
N      -0.13735  1.20343 -0.04121
C      -1.18645  1.23477 -1.03899
H      -0.85677  1.87942 -1.86088
C      -1.4666  -0.16617 -1.60995
C      -2.47779  1.85963 -0.52434
H      -2.1962  -0.08484 -2.41136
H      -0.53592 -0.53461 -2.04496
C      -1.98321 -1.13825 -0.60205
O      -2.25898  2.85111  0.35639
N      -1.3105  -1.43025  0.58173
C      -3.14012 -1.8589  -0.61502
C      -2.04897 -2.30198  1.25367
N      -3.16054 -2.58607  0.55483
H      -3.94171 -1.89228 -1.32841
H      -1.81759 -2.7267  2.21405
O      -3.57801  1.52886 -0.88772
H      2.26358  0.6946  2.58587
H      -3.8922  -3.21195  0.84843
```

H	3.146	-3.06122	-2.02447
H	0.95267	1.66548	2.55193
H	-3.12149	3.24093	0.56543
Ca	0.37233	-0.72035	1.37049

## 11.4 d Im[NNNN]<sub>OH</sub>



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

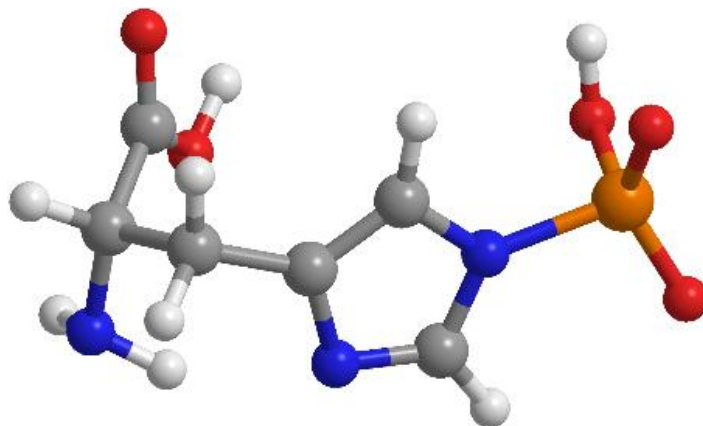
### Kartesische Koordinaten (XYZ Format)

```
N      1.417  0.61959  2.13223
C      1.94609  1.58407  1.12099
H      2.28902  2.49741  1.60376
C      3.14253  0.96123  0.39076
C      0.81872  1.974  0.15333
H      3.51888  1.70509 -0.31037
H      3.94052  0.80423  1.1231
C      2.89471 -0.32299 -0.3491
O      0.84184  3.0858 -0.38764
N      1.86646 -1.21257 -0.06254
C      3.63619 -0.85385 -1.3653
C      1.98639 -2.24039 -0.88613
N      3.05199 -2.05953 -1.68408
H      4.50754 -0.48701 -1.8753
H      1.3298 -3.09032 -0.93339
N      -0.09285  1.01913 -0.02644
C      -1.08708  1.19952 -1.08081
H      -0.61398  1.73426 -1.91053
C      -1.57551 -0.14951 -1.6178
C      -2.24615  2.08184 -0.5909
H      -2.33409  0.03712 -2.37411
H      -0.73134 -0.63136 -2.11693
C      -2.14074 -1.08695 -0.60617
O      -1.89025  3.32266 -0.25725
N      -1.3891 -1.58455  0.45438
C      -3.38869 -1.62606 -0.52629
C      -2.17493 -2.39748  1.15068
N      -3.3881 -2.44725  0.57952
H      -4.26301 -1.47129 -1.1294
H      -1.90453 -2.94082  2.03819
O      -3.38047  1.68974 -0.50926
H      2.17945  0.20335  2.65814
H      -4.17044 -2.9848  0.91498
H      3.36786 -2.69839 -2.39528
```

H	-0.92598	3.45925	-0.40385
H	0.83862	1.11773	2.8023
Ca	0.35053	-1.03085	1.22039

12 [pHis]<sup>-</sup>

### 12.1 Konformer a

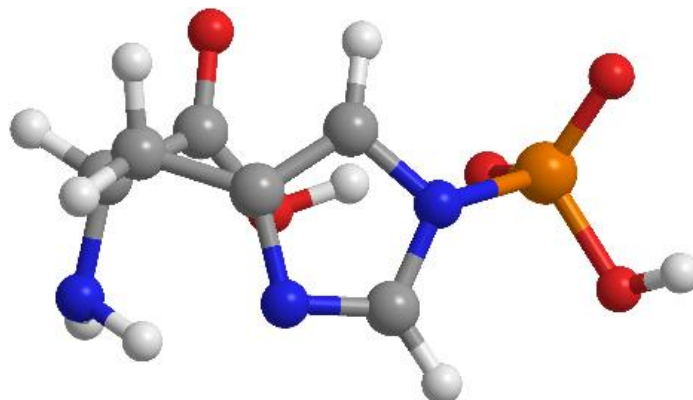


opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

N	-1.267	-1.594	-0.583
C	-2.423	-1.249	0.245
C	-3.709	-1.748	-0.429
C	-3.77	-3.262	-0.393
C	-4.748	-4.009	0.207
N	-4.363	-5.327	0.041
P	-5.217	-6.707	0.625
O	-4.672	-7.013	2.084
O	-6.702	-6.277	0.873
O	-4.893	-7.946	-0.274
C	-3.214	-5.338	-0.658
N	-2.801	-4.094	-0.937
C	-2.284	-1.851	1.653
O	-1.129	-2.496	1.782
O	-3.087	-1.765	2.536
H	-2.467	-0.164	0.342
H	-0.533	-1.77	0.092
H	-1.501	-2.518	-0.946
H	-4.569	-1.346	0.108
H	-3.752	-1.404	-1.464
H	-5.63	-3.658	0.724
H	-5.133	-6.378	2.631
H	-2.684	-6.236	-0.943
H	-1.145	-2.966	2.617

## 12.2 Konformer b



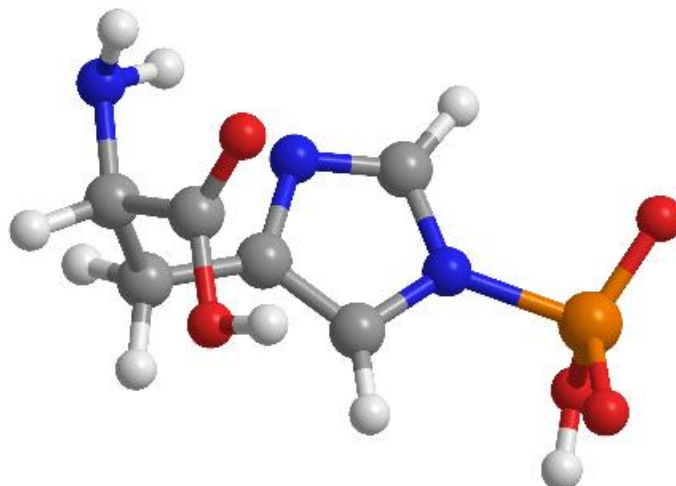
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	-1.07	-2.141	-0.35
C	-2.158	-1.515	0.403
C	-3.431	-1.479	-0.468
C	-3.92	-2.904	-0.596
C	-4.756	-3.523	0.291
N	-4.511	-4.87	0.118
P	-4.647	-6.015	1.39
O	-4.313	-7.466	0.844
O	-3.53	-5.581	2.403
O	-6.141	-6.077	1.848
C	-3.777	-5.014	-1.002
N	-3.401	-3.826	-1.492
C	-2.409	-2.29	1.714
O	-1.897	-3.516	1.628
O	-3.043	-1.884	2.645
H	-1.865	-0.496	0.657
H	-0.599	-2.702	0.352
H	-1.54	-2.837	-0.925
H	-4.195	-0.878	0.027
H	-3.22	-1.056	-1.45
H	-5.225	-3.073	1.155
H	-5.148	-7.769	0.486
H	-3.434	-5.963	-1.389
H	-2.406	-4.151	2.158



## 12.3 Konformer c



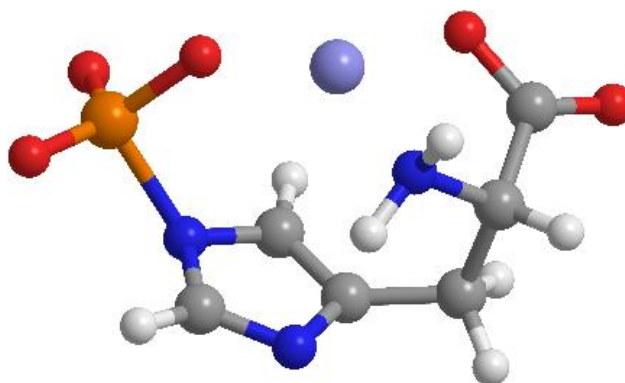
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	-1.852	-1.237	-1.028
C	-2.447	-1.152	0.302
C	-3.899	-1.653	0.251
C	-3.942	-3.156	0.061
C	-4.568	-4.045	0.892
N	-4.302	-5.296	0.367
P	-4.809	-6.798	1.045
O	-6.125	-7.251	0.283
O	-3.71	-7.883	0.792
O	-5.306	-6.507	2.501
C	-3.549	-5.13	-0.736
N	-3.304	-3.833	-0.97
C	-1.575	-1.971	1.259
O	-2.199	-2.201	2.402
O	-0.467	-2.357	1.009
H	-2.434	-0.11	0.624
H	-0.864	-1.375	-0.851
H	-2.182	-2.137	-1.377
H	-4.398	-1.4	1.187
H	-4.436	-1.168	-0.565
H	-5.127	-3.832	1.791
H	-6.81	-6.715	0.682
H	-3.185	-5.941	-1.351
H	-1.693	-2.836	2.91

## 13 [Ni<sup>2+</sup>(pHis)]<sup>-</sup>

### 13.1 Konformer a

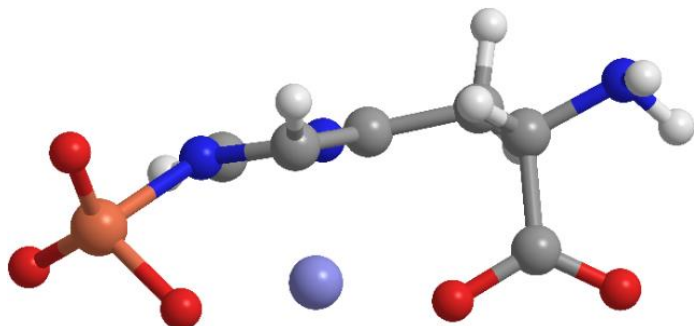


opt freq b3lyp/cc-pvtz geom=connectivity

#### Kartesische Koordinaten (XYZ Format)

C	-0.29116	3.14188	2.93441
C	-0.00384	2.48881	1.76652
C	0.76059	4.49359	1.5369
H	-0.77716	2.78846	3.82609
H	1.2215	5.39878	1.17259
N	0.19891	4.43859	2.79959
N	0.66073	3.35697	0.90243
C	-0.31169	1.07442	1.37283
H	0.46503	0.59551	0.76353
H	-0.45731	0.43629	2.24723
C	-1.61376	1.28892	0.57783
C	-3.03416	0.54657	0.72483
O	-2.95417	-0.68756	0.88611
O	-4.01412	1.31272	0.67336
P	0.0995	5.73399	3.92634
O	0.54165	5.11658	5.33867
O	0.80595	6.91278	3.38175
O	-1.45065	5.85699	4.32266
N	-1.60998	2.65288	0.02965
H	-0.67091	2.99457	-0.00757
H	-1.9978	2.64277	-0.89203
H	-1.32279	0.68982	-0.25962
Ni	-2.27842	4.59259	-0.01997

## 13.2 Konformer b



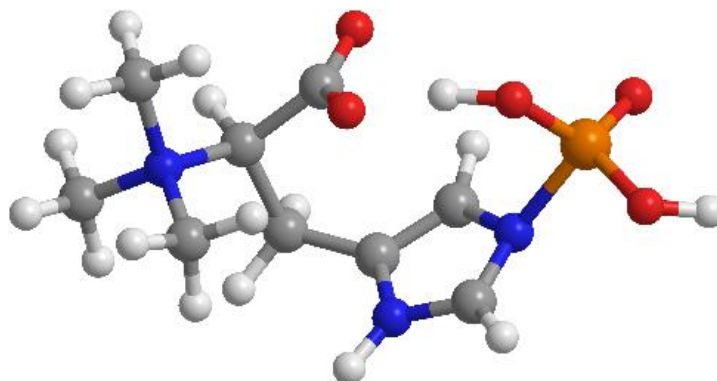
opt freq b3lyp/cc-pvtz geom=connectivity

### Kartesische Koordinaten (XYZ Format)

C	1.08819	2.42099	3.00675
C	0.69673	2.01501	1.78615
C	1.98918	3.78783	1.42747
H	0.69111	2.07294	3.93739
H	2.38294	4.68116	0.98949
N	2.14178	3.42355	2.84976
N	1.30623	2.88924	0.77263
C	-0.2512	0.83631	1.49683
H	0.22368	0.68881	0.54939
H	0.09774	-0.16267	1.6555
C	-1.53157	1.09504	0.68117
C	-1.78379	2.61144	0.58889
O	-1.4048	3.37005	1.51865
O	-2.36887	3.09195	-0.41628
P	1.97842	4.78091	3.94219
O	2.09394	4.28117	5.41132
O	3.06791	5.78137	3.66555
O	0.59103	5.45305	3.73051
N	-1.37116	0.54179	-0.67127
H	-2.18178	0.00762	-0.91121
H	-1.2587	1.28924	-1.326
H	-2.36271	0.62391	1.16299
Ni	-0.28173	4.05399	2.42947

## 14 [pHercynin]<sup>+</sup>

### 14.1 Konformer a



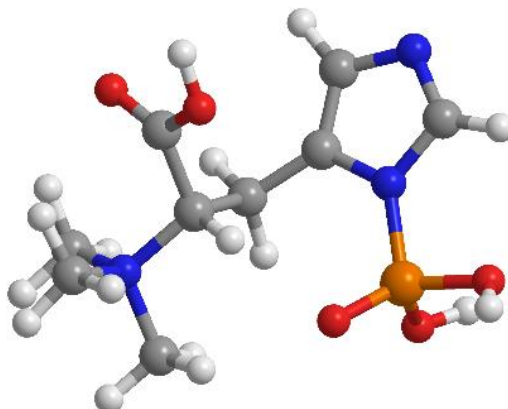
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

```
O      2.46231  1.84719 -1.32256
C      2.26348  1.67461 -0.15083
O      1.79557  2.61638  0.674
C      2.5504   0.39548  0.64285
C      1.39336  0.02982  1.5963
C      0.07761 -0.309   0.98335
C     -1.00162  0.4951   0.76819
N     -1.9786  -0.32152  0.21501
P     -3.54717  0.21928 -0.23016
O     -4.56068 -0.73015  0.55574
O     -3.59079 -0.39153 -1.69626
O     -3.68539  1.6599  -0.00695
C     -1.4355  -1.581   0.12732
N     -0.20858 -1.60429  0.57673
N      3.07267 -0.73504 -0.25856
C      4.44422 -0.35822 -0.75783
C      3.20227 -1.9964  0.55362
C      2.19591 -1.05423 -1.4505
H      3.40507  0.63357  1.27803
H      1.28177  0.90129  2.23668
H      1.70813 -0.78322  2.24568
H     -1.19159  1.53602  0.95345
H     -4.96116 -0.30011  1.32241
H     -4.44722 -0.32174 -2.13733
H     -1.9853  -2.41676 -0.26975
H      5.09872 -0.2092  0.09629
H      4.81614 -1.17563 -1.36724
H      4.36823  0.54482 -1.35011
H      2.21036 -2.36634  0.7908
H      3.73477 -2.72258 -0.05229
```

H	3.76993	-1.78509	1.45543
H	1.22768	-1.37423	-1.08801
H	2.67865	-1.86771	-1.98406
H	2.12285	-0.17881	-2.07938
H	0.40097	-2.39591	0.619

## 14.2 Konformer b



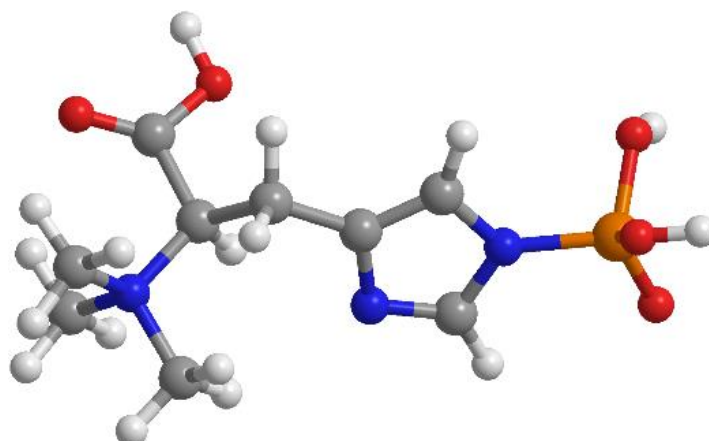
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

O	2.945	0.461	1.754
C	1.776	0.218	1.724
O	0.938	0.508	2.706
C	1.035	-0.444	0.553
C	1.688	-1.804	0.225
C	1.637	-2.719	1.437
C	2.593	-2.789	2.417
N	2.166	-3.694	3.372
C	0.998	-4.182	2.947
N	0.638	-3.625	1.774
P	-0.803	-4.005	0.901
O	-0.439	-4.509	-0.56
O	-1.662	-5.19	1.508
O	-1.616	-2.779	0.758
N	0.911	0.49	-0.62
C	0.323	1.786	-0.175
C	2.216	0.772	-1.278
C	-0.011	-0.084	-1.638
H	0.023	-0.665	0.897
H	1.416	0.853	3.468
H	2.738	-1.666	-0.036
H	1.19	-2.306	-0.601
H	3.509	-2.218	2.457
H	0.42	-4.925	3.479
H	-0.001	-5.356	-0.445
H	-2.544	-5.105	1.142
H	-0.613	1.617	0.361
H	0.111	2.426	-1.033
H	1.002	2.338	0.476
H	2.925	1.241	-0.596
H	2.664	-0.139	-1.676
H	2.069	1.456	-2.115

H	-0.205	0.64	-2.431
H	-0.967	-0.354	-1.186
H	0.413	-0.968	-2.112

### 14.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

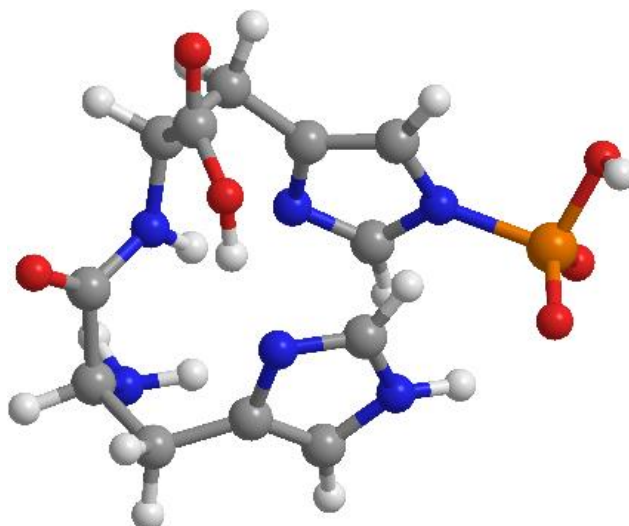
O	4.367	-1.055	2.612
C	3.705	-0.945	1.621
O	4.218	-0.734	0.418
C	2.17	-0.975	1.57
C	1.644	-2.091	2.499
C	2.296	-3.402	2.121
C	2.624	-4.415	2.983
N	3.198	-5.398	2.193
P	3.831	-6.906	2.748
O	2.838	-8.097	2.412
O	3.837	-6.933	4.336
O	5.19	-7.169	2.238
C	3.2	-4.963	0.919
N	2.657	-3.744	0.83
N	1.585	0.383	1.838
C	0.101	0.326	1.751
C	1.959	0.919	3.175
C	2.054	1.347	0.803
H	1.88	-1.26	0.556
H	5.176	-0.807	0.448
H	0.57	-2.23	2.387
H	1.88	-1.882	3.542
H	2.478	-4.447	4.054
H	2.013	-7.888	2.852
H	4.439	-7.642	4.575
H	3.592	-5.521	0.08
H	-0.326	1.329	1.793
H	-0.212	-0.138	0.814
H	-0.324	-0.237	2.582
H	3.037	1.049	3.273
H	1.498	1.897	3.323



H	1.613	0.268	3.977
H	1.848	0.966	-0.199
H	3.123	1.544	0.89
H	1.543	2.305	0.912

## 15 [pHisHis]<sup>-</sup>

### 15.1 Konformer a



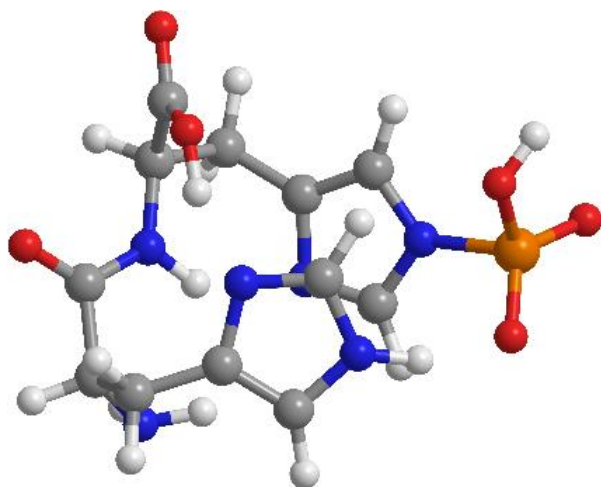
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

N	-2.547	-1.417	-0.133
C	-3.736	-0.564	-0.076
C	-3.796	0.215	1.25
C	-2.625	1.136	1.486
C	-1.365	0.863	1.954
N	-0.636	2.038	1.864
C	-1.466	2.986	1.405
N	-2.677	2.483	1.156
C	-3.735	0.339	-1.31
N	-2.649	1.086	-1.467
C	-2.22	1.739	-2.694
C	-0.941	1.038	-3.182
C	0.039	0.902	-2.035
C	0.988	1.818	-1.669
N	1.562	1.311	-0.515
P	2.758	2.083	0.454
O	3.141	3.455	-0.245
O	2.033	2.511	1.775
O	4.034	1.181	0.517
C	1.006	0.113	-0.265
N	0.039	-0.167	-1.147
C	-1.966	3.23	-2.447
O	-2.664	3.671	-1.407
O	-1.247	3.933	-3.101
O	-4.643	0.291	-2.131
H	-4.617	-1.206	-0.122

H	-2.983	1.654	-3.468
H	-1.725	-0.834	-0.292
H	-2.623	-1.976	-0.971
H	-4.711	0.809	1.26
H	-3.846	-0.496	2.075
H	-0.991	-0.104	2.259
H	0.365	2.166	2.033
H	-1.178	4.012	1.223
H	-1.966	1.066	-0.722
H	-1.197	0.04	-3.539
H	-0.487	1.595	-4.002
H	1.217	2.762	-2.144
H	2.453	4.061	0.029
H	1.273	-0.518	0.571
H	-2.976	2.94	-0.857

## 15.2 Konformer b



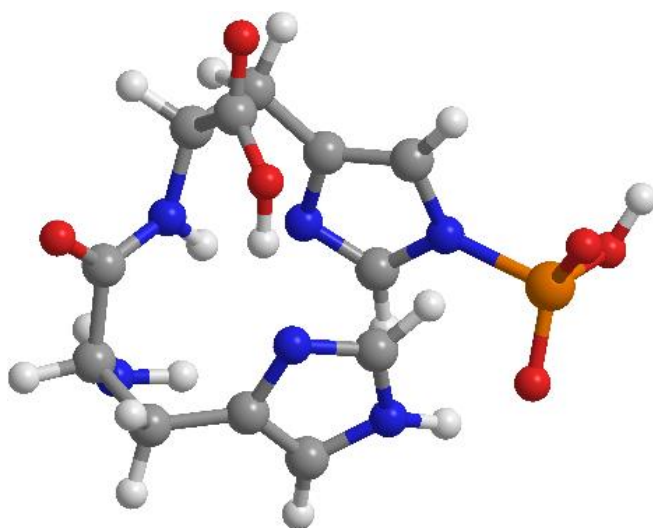
opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

### Kartesische Koordinaten (XYZ Format)

N	-2.593	-1.392	-0.072
C	-3.776	-0.531	-0.034
C	-3.818	0.299	1.262
C	-2.604	1.164	1.49
C	-1.387	0.853	2.04
N	-0.585	1.975	1.909
C	-1.325	2.93	1.328
N	-2.556	2.484	1.062
C	-3.781	0.323	-1.303
N	-2.71	1.085	-1.483
C	-2.287	1.696	-2.733
C	-1.002	0.99	-3.197
C	-0.026	0.879	-2.044
C	0.894	1.823	-1.671
N	1.487	1.324	-0.523
P	2.662	2.132	0.442
O	2.709	3.649	-0.017
O	2.12	2.175	1.912
O	4.087	1.558	0.154
C	0.957	0.114	-0.273
N	0.003	-0.192	-1.159
C	-2.051	3.2	-2.551
O	-2.695	3.666	-1.488
O	-1.39	3.893	-3.274
O	-4.68	0.219	-2.13
H	-4.662	-1.167	-0.049
H	-3.049	1.572	-3.503
H	-1.77	-0.813	-0.245
H	-2.672	-1.966	-0.899
H	-4.703	0.937	1.238

H	-3.915	-0.382	2.109
H	-1.088	-0.11	2.43
H	0.415	2.053	2.115
H	-0.961	3.916	1.08
H	-2.037	1.119	-0.728
H	-1.253	-0.016	-3.532
H	-0.545	1.529	-4.028
H	1.094	2.778	-2.135
H	3.461	4.008	0.454
H	1.236	-0.51	0.564
H	-2.953	2.951	-0.89

### 15.3 Konformer c



opt freq b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj int=ultrafine pop=regular

#### Kartesische Koordinaten (XYZ Format)

N	-2.411	-1.418	-0.133
C	-3.66	-0.655	-0.095
C	-3.789	0.134	1.22
C	-2.66	1.099	1.483
C	-1.422	0.884	2.033
N	-0.725	2.077	1.94
C	-1.548	2.979	1.388
N	-2.731	2.431	1.095
C	-3.713	0.227	-1.342
N	-2.701	1.073	-1.489
C	-2.31	1.745	-2.717
C	-0.967	1.153	-3.178
C	0.001	1.096	-2.014
C	0.856	2.091	-1.624
N	1.467	1.621	-0.473

P	2.569	2.497	0.518
O	3.918	1.672	0.612
O	2.947	3.817	-0.231
O	1.94	2.561	1.952
C	1.002	0.383	-0.231
N	0.085	0.022	-1.136
C	-2.192	3.258	-2.495
O	-2.896	3.647	-1.438
O	-1.568	4.015	-3.184
O	-4.591	0.076	-2.185
H	-4.492	-1.36	-0.141
H	-3.05	1.583	-3.502
H	-1.635	-0.772	-0.277
H	-2.432	-1.977	-0.973
H	-4.726	0.692	1.2
H	-3.834	-0.572	2.049
H	-1.038	-0.059	2.397
H	0.263	2.241	2.157
H	-1.277	4.003	1.175
H	-2.041	1.137	-0.724
H	-1.134	0.137	-3.537
H	-0.545	1.744	-3.991
H	1.002	3.062	-2.079
H	4.375	1.889	-0.201
H	1.304	-0.226	0.609
H	-3.114	2.901	-0.864

# 16 NMR Spektren Hercynin und *N* $\epsilon$ -Methyl-Hercynin

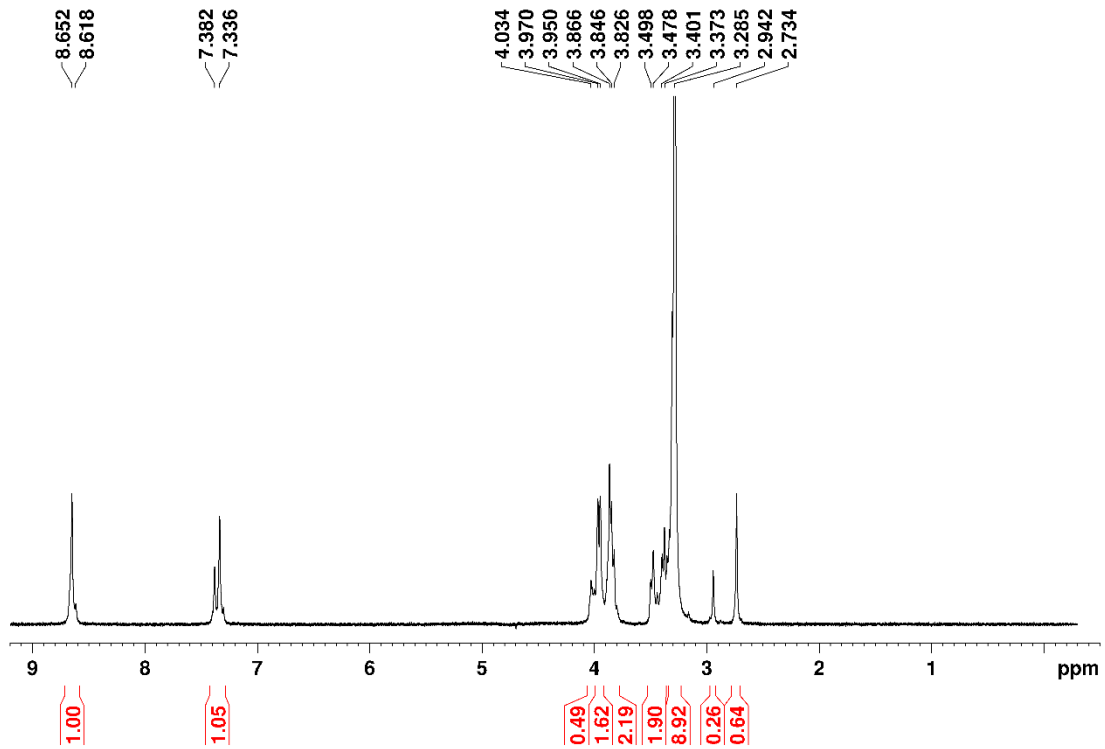
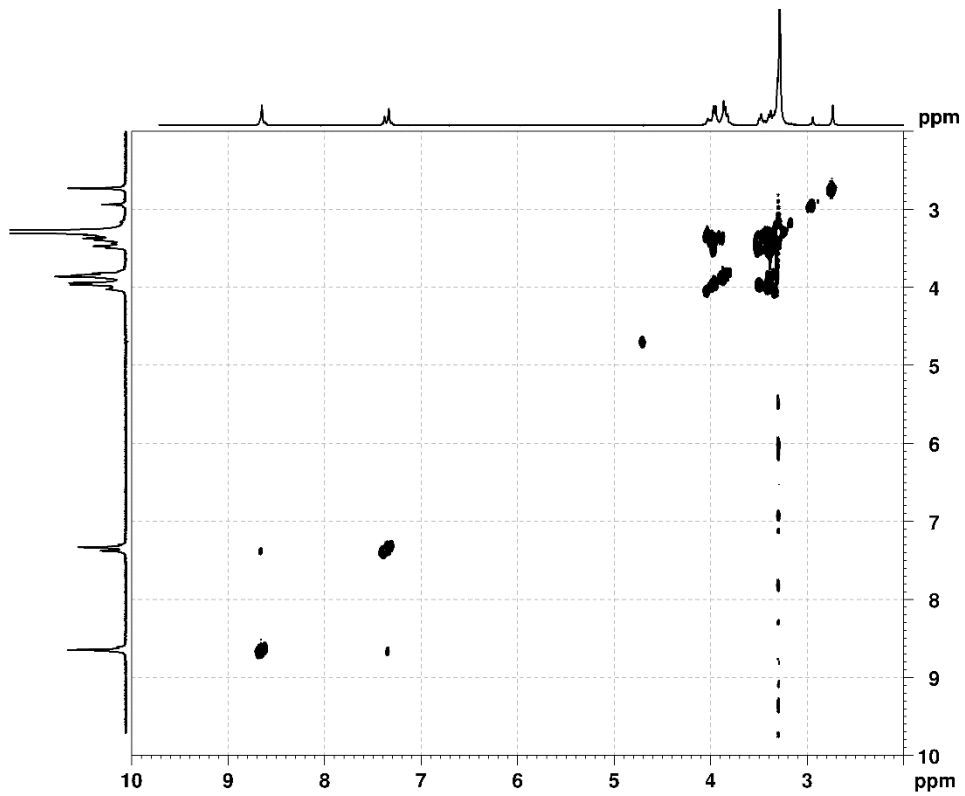
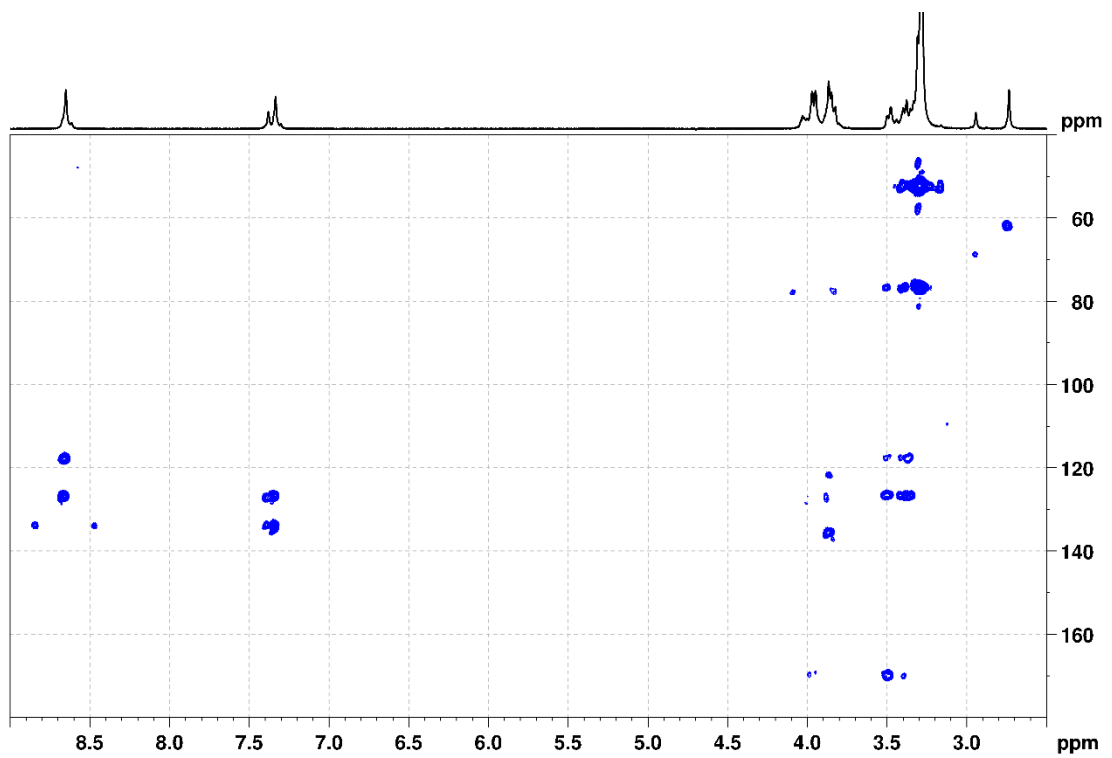


Abbildung 1.  $^1\text{H}$  NMR Spektrum von Hercynin und *N* $\epsilon$ -Methyl-Hercynin (600 MHz,  $\text{D}_2\text{O}$ , 298K).

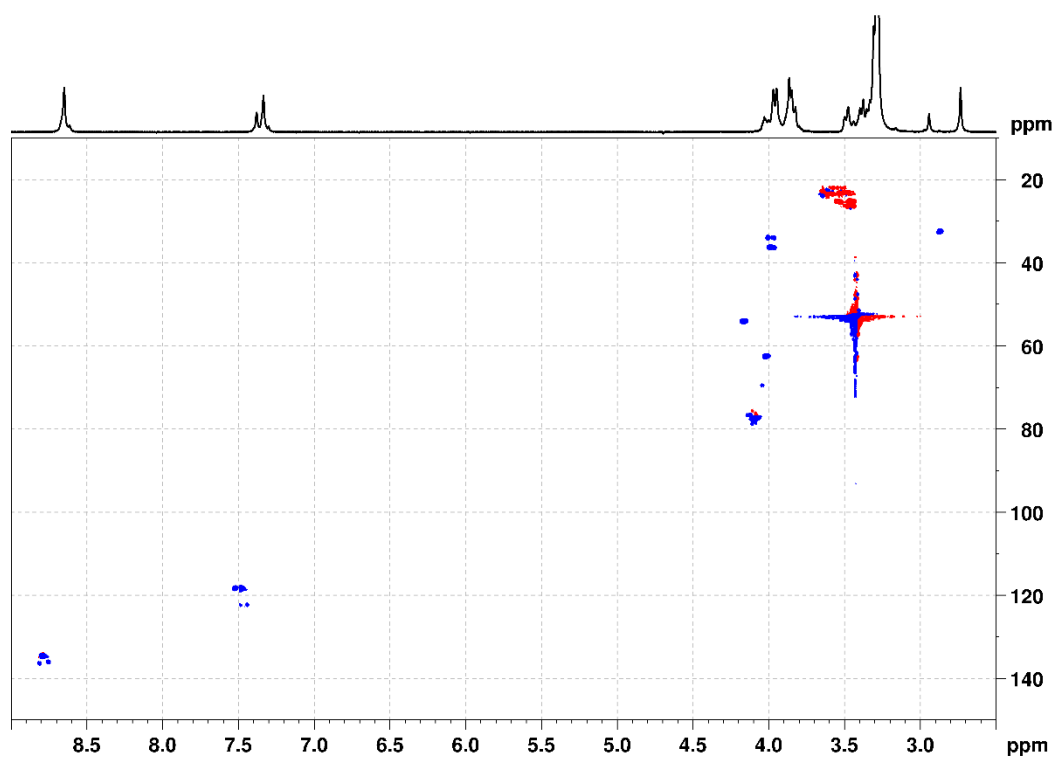


**Abbildung 2.**  $^1\text{H}, ^1\text{H}$  COSY NMR Spektrum von Hercynin und *N* $\epsilon$ -Methyl-Hercynin (600 MHz,  $\text{D}_2\text{O}$ , 298K).





**Abbildung 3.**  $^1\text{H}$  (600 MHz),  $^{13}\text{C}$  (151 MHz) HMBC NMR Spektrum von Hercynin und *Ne*-Methyl-Hercynin (600 MHz,  $\text{D}_2\text{O}$ , 298K).



**Abbildung 4.**  $^1\text{H}$  (600 MHz),  $^{13}\text{C}$  (151 MHz) HSQC NMR Spektrum von Hercynin und *N* $\epsilon$ -Methyl-Hercynin (600 MHz,  $\text{D}_2\text{O}$ , 298K).

## 17 Genehmigung zum Abdruck durch ACS



RightsLink®

Home

Create Account

Help



ACS Publications  
Most Trusted. Most Cited. Most Read.

**Title:** Hydrogen Tunneling above Room Temperature Evidenced by Infrared Ion Spectroscopy  
**Author:** Mathias Schäfer, Katrin Peckelsen, Mathias Paul, et al  
**Publication:** Journal of the American Chemical Society  
**Publisher:** American Chemical Society  
**Date:** Apr 1, 2017  
Copyright © 2017, American Chemical Society

LOGIN

If you're a [copyright.com](#) user, you can login to RightsLink using your [copyright.com](#) credentials. Already a [RightsLink](#) user or want to [learn more?](#)

### PERMISSION/LICENSE IS GRANTED FOR YOUR ORDER AT NO CHARGE

This type of permission/license, instead of the standard Terms & Conditions, is sent to you because no fee is being charged for your order. Please note the following:

- Permission is granted for your request in both print and electronic formats, and translations.
- If figures and/or tables were requested, they may be adapted or used in part.
- Please print this page for your records and send a copy of it to your publisher/graduate school.
- Appropriate credit for the requested material should be given as follows: "Reprinted (adapted) with permission from (COMPLETE REFERENCE CITATION). Copyright (YEAR) American Chemical Society." Insert appropriate information in place of the capitalized words.
- One-time permission is granted only for the use specified in your request. No additional uses are granted (such as derivative works or other editions). For any other uses, please submit a new request.

BACK

CLOSE WINDOW

Copyright © 2018 [Copyright Clearance Center, Inc.](#) All Rights Reserved. [Privacy statement](#). [Terms and Conditions](#). Comments? We would like to hear from you. E-mail us at [customer@copyright.com](mailto:customer@copyright.com)