Refcode	S(OC)	S(TPR)	α	Δ	d_1	d_2
GITTAE	13.68	0.92	67	0.79	2.828	2.331
Lyonsite	17.57	1.18	61	0.94	2.575	2.575
HENQIA	12.43	2.24	68	0.81	2.321	2.250
Buttgenbachite	19.01	2.94	58	0.95	2.910	2.910
DUYJEM	6.97	3.59	77	0.34	2.266	2.254
BOTHOH	5.75	3.73	76	0.22	2.205	2.197
VIFKAW	5.34	3.85	78	0.19	2.263	2.263
RINKII	5.31	3.87	82	0.12	2.184	2.135
NELHAN	5.67	3.93	76	0.26	2.347	2.295
ACADIS-Cu1	5.70	4.28	73	0.24	2.239	2.211
AWENEV	4.88	4.83	73	0.31	2.320	2.205
JEXZOC	4.45	5.08	76	0.22	2.259	2.139
BAFMOK	20.51	5.93	67	0.65	2.645	2.645
ETUFAA-Cu1	4.09	6.46	73	0.27	2.293	2.150
NEENCU	19.23	7.34	82	0.51	2.509	2.509
LOTSOC	2.40	8.27	78	0.19	2.218	2.211
ETAMCU	2.42	9.26	84	0.26	2.265	2.235
AHICOJ	2.87	9.44	70	0.32	2.286	2.209
AHICID	2.49	10.16	71	0.31	2.291	2.236
HIGSUM	1.70	10.31	79	0.23	2.247	2.197
XAGWAE	1.65	11.63	89	0.10	2.179	2.175
UFAPOH	1.37	11.74	81	0.10	2.172	2.169
FUPJIJ-Cu1	1.33	12.31	97	0.15	2.200	2.165
CEYLAU	0.77	14.20	105	0.20	2.182	2.182
KOJTOS01	0.60	15.18	81	0.42	2.403	2.243

Table S1. Shape and geometrical parameters for *cis*-distorted Cu(II) complexes with N- or O-donor ligands. S(OC) and S(TPR) are the octahedral and trigonal prismatic shape measures, respectively, α is the L-M-L bond angle between the two longest M-L bonds, d_1 and d_2 are the two longest M-L distances and Δ is the difference between the longest and shortest M-L bond distances. All distances in Å, angles in degrees.

Refcode	S(OC)	S(TPR)	α	Δ
PURZIL	12.83	0.92	131	0.232
ACADIS-Cu2	5.78	3.95	152	0.119
ZALFUN	4.97	4.11	152	0.210
ZOVFIZ	6.43	4.99	137	0.444
KELZOQ	5.63	5.36	160	0.475
CALCEY	5.39	5.41	151	0.507
SECBAE	4.15	7.18	149	0.438
ETUFAA-Cu2	3.48	7.18	153	0.273
ECEZUH	4.35	7.33	148	0.599
PIWTAQ	4.20	7.42	160	0.418
MEMYUY	2.91	7.87	151	0.370
EBOGOS01	3.32	8.07	154	0.533
EBOGOS	3.37	8.14	154	0.547
RIJTOT	3.38	8.18	153	0.513
LERZUE	3.33	8.71	155	0.336
AXOKON-Cu3	3.17	8.97	161	0.279
QEZKEM	2.18	9.65	156	0.394
KOSYUM	2.45	10.16	154	0.444
PIKZOZ	2.37	10.23	162	0.454
GAZVEI	1.67	10.71	176	0.269
ZIZPUT	1.85	10.81	161	0.442
EXIWEN	1.33	10.94	166	0.275
KCUEDA10	2.06	10.99	173	0.451
DIVZIR	1.49	11.02	179	0.290
SIHMUR	1.50	11.18	168	0.373
WUTXAK-Cu3	1.550	11.24	169	0.213
LUHNUX-Cu2	1.600	11.30	163	0.336
XUTYOA	1.61	11.32	166	0.269
CMGEDT01	1.60	11.51	176	0.306
IROMAD	1.65	11.70	156	0.385
BIWCOZ01	1.15	11.78	164	0.196
EBUYIJ	1.64	11.79	166	0.431
YENTAN-Cu2	1.40	11.90	169	0.152
AJOGAH	1.56	12.20	162	0.364
YENTAN-Cu1	1.36	12.23	169	0.176
GUMPEJ	1.41	12.44	172	0.404
ROSHOW	1.34	12.68	169	0.379
LIZVIZ	1.23	12.71	166	0.382
MUSREX	1.34	12.82	169	0.283
HEFZIC	1.22	12.85	172	0.107
QELRAB	1.38	12.87	172	0.310
REZJAI	1.32	12.99	170	0.137

LUHNUX-Cu1	1.22	13.22	169	0.380
QILFEW	1.07	13.50	171	0.311
KEQRAZ	1.04	13.58	171	0.298
NEGRUN	0.88	13.58	172	0.097
FECQEK-Cu3	0.40	13.59	169	0.139
PUSGEP	0.98	13.60	165	0.330
CEYLUO-Cu1	0.90	13.69	154	0.772
UDOBOE	1.00	13.73	176	0.369
HEWQUW	0.43	13.81	175	0.076
YUDNAM	1.05	13.89	175	0.334
TUXZUH	0.64	14.19	172	0.244
FACPCU	0.69	14.71	167	0.307
PUSGEP-Cu1	0.49	14.81	175	0.267
NAFACU10	0.30	15.12	175	0.222
CDSRCA10	0.72	15.14	172	0.367
MEGPEU	0.53	15.26	175	0.309
ISIPIJ-Cu2	0.37	15.33	174	0.247
HOKJIA	0.26	15.37	180	0.178
KIXKIL	0.56	15.57	176	0.302
TFAPCU01	0.59	15.64	173	0.328
CUETNM10	0.43	15.68	175	0.396
JURXEZ	0.37	15.83	177	0.296
DUBTAV	0.21	15.88	177	0.254
TFAPCU	0.55	15.93	173	0.324
RECCOS	0.49	15.97	180	0.226
GIKCEJ	0.51	16.01	180	0.159
GIKSUO01	0.45	16.05	180	0.290
RELCUG04	0.37	16.07	180	0.190
CAMSCU	0.41	16.07	179	0.257
KUKFOL	0.46	16.08	180	0.236
YAGDIU	0.09	16.15	180	0.086
TAFACU-Cu1	0.06	16.18	178	0.089
PEVDAW	0.20	16.19	180	0.116
VENNUY	0.05	16.21	180	0.022
HOKJEW	0.49	16.23	180	0.319
FOFKAN	0.11	16.24	180	0.115
MIGGIT	0.38	16.26	180	0.228
PIJSIL	0.40	16.26	180	0.291
ZODHUV	0.23	16.34	180	0.189
MINZAK	0.19	16.38	180	0.192
PANNIC	0.42	16.39	180	0.296
BECXAJ	0.10	16.41	180	0.119
PABREQ	0.06	16.45	180	0.093

RIDMUN	0.21	16.48	180	0.197
DAZKOF	0.44	16.48	180	0.269
TAFACU-Cu2	0.44	16.48	178	0.300
AVUJEG02	0.07	16.51	180	0.141
QESXER	0.32	16.57	180	0.238
HOYZEA	0.24	16.57	180	0.232
REFGAL	0.32	16.58	180	0.230
ZUBKOW01	0.10	16.59	180	0.150
VUDRER05	0.24	16.60	180	0.222
ZUBKOW-Cu2	0.05	16.63	180	0.108
YIGMOQ	0.29	16.66	180	0.238
FAHHOL	0.17	16.66	180	0.199
HOYZIE-Cu1	0.15	16.71	180	0.193
VUDRER04	0.35	16.71	180	0.272

Table S2. Shape and geometrical parameters for *trans*-distorted Cu(II) complexes with N- or O-donor ligands. S(OC) and S(TPR) are the octahedral and trigonal prismatic shape measures, respectively, α is the L-M-L bond angle between the two longest M-L bonds (in degrees), and Δ is the difference between the longest and shortest M-L bond distances (Å).

Table S3. Atomic coordinates of the optimized structure of $[Cu(\mathbf{1})]^{2+}$.

61			
C	-2.843747	-0.427418	-0.215283
C	-2.064645	-1.625850	-0.791293
C	-2.706893	-2.831913	-1.068117
C	-1.961175	-3.893541	-1.574453
C	-0.600861	-3.731452	-1.812499
C	-0.001054	-2.508892	-1.511145
C	1.417158	-2.189401	-1.775672
C	2.288160	-3.051458	-2.444856
C	3.584395	-2.632617	-2.732458
C	3.980827	-1.350010	-2.361845
C	3.073343	-0.540208	-1.687855
C	-2.529631	0.899548	-0.934677
C	-3.520232	1.706615	-1.493468
C	-3.153610	2.936459	-2.038369
C	-1.833270	3.371266	-1.954905
C	-0.891145	2.538888	-1.351095
C	0.499919	2.917890	-1.024788
C	1.047485	4.169827	-1.304282
C	2.318553	4.487639	-0.831842
C	3.012330	3.552183	-0.068408
C	2.427704	2.311868	0.162899
C	-2.474917	-0.273592	1.274656
C	-3.433267	-0.197439	2.278683
C	-2.978187	-0.081188	3.592811
C	-1.612596	-0.089693	3.861433
C	-0.705405	-0.191605	2.798966
C	0.763215	-0.348004	2.973015
C	1.356858	-0.447404	4.236859
C	2.719482	-0.709259	4.342077
C	3.466519	-0.885231	3.179968
C	2.819594	-0.755807	1.955383
Cu	0.321525	0.109403	-0.289493
H	-4.588039	-0.824785	-1.163856
H	-3.758304	-2.945538	-0.863113
H	-2.438520	-4.839974	-1.782303
H	-0.025086	-4.546375	-2.219931
H	1.965055	-4.033602	-2.750688
H	4.265165	-3.291033	-3.251680
H	4.969390	-0.980626	-2.587462
H	3.341057	0.460626	-1.391373
H	-4.554477	1.406475	-1.472957
H	-3.901770	3.569518	-2.492603
H	-1.561134	4.343553	-2.333120
H	0.489366	4.897582	-1.871699
H	2.749153	5.455685	-1.041843
H	3.985384	3.773197	0.342483
H	2.923920	1.563359	0.757529
H	-4.482640	-0.237676	2.040015
H	-3.686782	-0.004493	4.404628
H	-1.273258	-0.030658	4.882734
H	0.769156	-0.338249	5.134033
H	3.183557	-0.790912	5.314090
H	4.520140	-1.116925	3.218272
H	3.363177	-0.890045	1.031585
N	-0.734897	-1.492590	-0.981699
N	1.820211	-0.944623	-1.386927
N	-1.251140	1.310674	-0.902416
N	1.207271	1.984806	-0.315389

N	-1.156880	-0.243217	1.526602
N	1.502546	-0.478499	1.836714
O	-4.259744	-0.688606	-0.252787

Table S4. Atomic coordinates of the optimized structure of $[Cu(\mathbf{2}\text{-pyridyl}_2)]^{2+}$.

63			
C	-1.229211	-2.295357	-1.865141
C	-0.096038	-1.817159	-2.763218
C	1.862733	-2.289877	-1.346414
C	2.660637	-1.776352	-0.153272
C	1.322340	-2.347791	1.836836
C	0.177151	-1.946803	2.767014
C	-1.761459	-2.397196	1.327610
C	-2.555052	-1.810252	0.168254
C	1.857568	-0.351757	-2.860246
C	-2.478980	-0.167654	-1.651764
C	-2.585577	1.070133	-0.801169
C	-3.704000	1.897151	-0.780260
C	-3.700869	3.022901	0.043222
C	-2.581147	3.287976	0.831573
C	-1.494107	2.426412	0.765946
C	2.430456	-0.152794	1.675562
C	2.498662	1.108264	0.853494
C	3.542213	2.024437	0.977300
C	3.532516	3.186235	0.210014
C	2.476880	3.407307	-0.675770
C	1.466272	2.462123	-0.759192
C	-1.836162	-0.579573	2.974155
Cu	0.008850	-0.102551	-0.202886
N	-1.685702	-1.220089	-0.919297
N	1.022430	-1.214828	-1.968006
N	1.761063	-1.250337	0.922007
N	-0.978605	-1.359626	2.043823
N	-1.488512	1.338857	-0.043743
N	1.468452	1.330014	-0.005572
H	-2.256665	-1.208866	3.768422
H	-1.250319	0.212282	3.437251
H	-2.659933	-0.114818	2.437264
H	-2.463401	-2.902579	2.005084
H	-1.083643	-3.167678	0.962487
H	-3.198258	-2.577869	-0.271779
H	-3.206824	-1.020901	0.534754
H	-2.068477	-2.636652	-2.479276
H	-0.913439	-3.147305	-1.266830
H	0.262915	-2.654650	-3.371384
H	-0.450086	-1.062405	-3.463696
H	-3.468336	-0.551520	-1.912532
H	-1.970126	0.071931	-2.585339
H	-4.563959	1.662312	-1.390391
H	-4.560083	3.676977	0.074405
H	-2.550553	4.143008	1.489322
H	-0.608655	2.591047	1.358925
H	1.253291	0.459904	-3.259586
H	2.686543	0.078357	-2.306945
H	2.261041	-0.930156	-3.696935
H	2.546696	-2.708589	-2.092438
H	1.209850	-3.100672	-1.028166
H	3.296588	-2.579882	0.232278

H	3.327885	-0.976539	-0.468955
H	2.164860	-2.693960	2.448286
H	1.027973	-3.193728	1.217249
H	-0.114936	-2.830696	3.350915
H	0.520228	-1.212007	3.494273
H	3.435479	-0.445400	1.998369
H	1.856973	0.051060	2.579735
H	4.352218	1.824260	1.663357
H	4.335595	3.903738	0.295971
H	2.439117	4.291683	-1.293127
H	0.630949	2.594114	-1.428960

Table S5. Atomic coordinates of the optimized structure of $[Cu(\mathbf{2}\text{-carboxylate}_2)]^{2+}$, isomer **A**.

55

C	0.982702	-2.489627	-1.309102
C	-0.982741	2.489705	-1.309029
C	0.479645	-2.869457	0.093417
C	-0.479657	2.869470	0.093498
C	-0.825317	-1.824606	1.924065
C	0.825328	1.824530	1.924083
C	-2.188641	-1.671514	1.215975
C	2.188641	1.671458	1.215976
C	2.704780	-0.757908	0.915673
C	-2.704773	0.757850	0.915678
C	1.611195	-1.437215	1.755663
C	-1.611187	1.437135	1.755681
C	2.990215	0.817954	-0.984079
C	-2.990201	-0.818000	-0.984085
C	4.496503	1.085857	-0.852600
C	-4.496501	-1.085852	-0.852624
Cu	0.000025	0.000037	-0.369365
H	1.142552	-3.619046	0.530261
H	-1.142554	3.619034	0.530397
H	-0.498041	-3.332341	-0.037651
H	0.498028	3.332359	-0.037563
H	-0.803609	-2.802489	2.422964
H	0.803624	2.802394	2.423015
H	-0.721877	-1.074264	2.704137
H	0.721890	1.074159	2.704128
H	-2.962266	-1.636038	1.996531
H	2.962280	1.635989	1.996518
H	-2.387158	-2.570537	0.633516
H	2.387138	2.570483	0.633513
H	3.013721	-1.427541	0.114241
H	-3.013701	1.427493	0.114249
H	3.578873	-0.621054	1.569572
H	-3.578874	0.621004	1.569569
H	1.377292	-0.825575	2.624607
H	-1.377270	0.825462	2.624597
H	2.801422	-0.016634	-1.656683
H	-2.801361	0.016572	-1.656695
H	-2.492503	-1.678540	-1.432169
H	2.492492	1.678467	-1.432188
N	0.341667	-1.681449	1.001867
N	-0.341664	1.681408	1.001881
N	-2.276489	-0.515887	0.297604
N	2.276490	0.515830	0.297600
O	0.652960	-1.281018	-1.700902

O	-0.653028	1.281104	-1.700872
O	1.622720	-3.328226	-1.974131
O	-1.622754	3.328343	-1.974014
H	4.708615	1.936231	-0.200351
H	5.031623	0.216768	-0.465838
H	4.911629	1.313172	-1.836078
H	-5.031606	-0.216729	-0.465920
H	-4.911617	-1.313212	-1.836095
H	-4.708643	-1.936184	-0.200327
H	-2.008773	2.385459	2.137465
H	2.008786	-2.385554	2.137405

Table S6. Atomic coordinates of the optimized structure of $[Cu(\mathbf{2}\text{-carboxylate}_2)]^{2+}$, isomer **B**.

49

C	1.549764	-1.520157	-1.770554
C	0.605811	-2.654556	-1.357654
C	-1.610997	-1.659730	-1.716467
C	-2.559248	-0.614427	-1.132772
C	-1.567168	1.563172	-1.733554
C	-0.620252	2.690216	-1.306027
C	1.593907	1.701503	-1.693786
C	2.544094	0.646798	-1.131506
C	-1.217977	-3.104818	0.239616
C	2.660338	-1.221042	0.429658
C	2.562265	-0.375749	1.708816
C	-2.648138	1.218581	0.473957
C	-2.544360	0.338548	1.728438
C	1.211404	3.110765	0.290404
Cu	0.006487	-0.020128	0.510643
N	1.838895	-0.583001	-0.649821
N	-0.627935	-2.143240	-0.721889
N	-1.848050	0.602668	-0.632021
N	0.617242	2.170102	-0.687538
O	1.397372	0.215212	1.869285
O	-1.381424	-0.262674	1.864739
H	1.596787	4.019095	-0.195955
H	0.459229	3.392532	1.024036
H	2.013210	2.625751	0.839198
H	2.193736	2.540123	-2.081265
H	1.048775	1.291013	-2.544388
H	3.288000	0.379513	-1.892307
H	3.090118	1.065011	-0.289246
H	2.481542	-1.953193	-2.158944
H	1.105919	-0.944910	-2.583401
H	0.388704	-3.271216	-2.242889
H	1.103615	-3.309144	-0.645260
H	3.706347	-1.323707	0.130066
H	2.268892	-2.212245	0.650669
H	-0.463482	-3.399589	0.965672
H	-2.019113	-2.631688	0.799323
H	-1.602340	-4.003420	-0.264592
H	-2.210330	-2.493685	-2.113649
H	-1.070516	-1.234508	-2.562755
H	-3.304607	-0.333544	-1.887431
H	-3.104337	-1.046979	-0.297093
H	-2.501568	2.005072	-2.106361
H	-1.129905	1.005290	-2.562130

H	-0.410244	3.322515	-2.182249
H	-1.114162	3.332136	-0.579636
H	-3.697055	1.342326	0.192351
H	-2.240792	2.197983	0.717267
O	3.537147	-0.289525	2.478649
O	-3.513378	0.234844	2.503550

Table S7. Atomic coordinates of the optimized structure of $[Cu(\mathbf{4})]^{2+}$. The vibrational analysis of this structure gave one negative frequency at 15 cm^{-1}.

53

C	-3.194149	-0.219227	0.004076
C	3.194145	0.219225	0.004425
C	-2.811906	-0.099265	1.493731
C	2.811716	0.098271	1.493947
C	-0.744455	-0.171508	2.923988
C	0.744194	0.169615	2.924103
C	-2.935501	1.070652	-0.803824
C	2.935612	-1.070106	-0.804387
C	-0.997380	2.641095	-1.188989
C	0.997509	-2.640370	-1.190401
C	2.613389	1.474742	-0.674508
C	-2.613304	-1.474290	-0.675618
C	0.510989	2.634742	-1.397577
C	-0.510848	-2.633929	-1.399079
Cu	0.000012	0.000116	-0.233681
H	-3.525569	0.559576	1.995651
H	3.525293	-0.560933	1.995513
H	2.916874	1.073012	1.974469
H	-2.917093	-1.074332	1.973588
H	-1.430280	1.403630	1.802470
H	1.430008	-1.404780	1.801533
H	-1.201822	0.189465	3.850299
H	1.201565	-0.191975	3.850171
H	-0.875023	-1.256419	2.913984
H	0.874766	1.254533	2.914814
H	-3.598136	1.090424	-1.671389
H	3.598257	-1.089196	-1.671959
H	-3.200261	1.937515	-0.197556
H	3.200455	-1.937379	-0.198740
H	-1.457267	0.938843	-2.245560
H	1.457417	-0.937583	-2.246098
H	-1.478974	3.294655	-1.920468
H	1.479146	-3.293575	-1.922170
H	-1.241415	3.032453	-0.200416
H	1.241485	-3.032215	-0.202006
H	3.168415	2.357945	-0.349193
H	-3.168362	-2.357713	-0.350950
H	2.741073	1.404685	-1.755117
H	-2.740860	-1.403531	-1.756196
H	-1.062323	-2.124627	0.520668
H	1.062261	2.124429	0.521955
H	0.919265	3.643840	-1.308387
H	-0.919114	-3.643078	-1.310426
H	0.755540	2.272549	-2.396839
H	-0.755339	-2.271238	-2.398175
N	-1.410231	0.388629	1.712626
N	1.409992	-0.389719	1.712371
N	-1.510246	1.234965	-1.270749
N	1.510376	-1.234204	-1.271439

N	-1.146397	-1.701808	-0.404440
N	1.146449	1.702104	-0.403366
H	-4.279745	-0.358343	-0.010823
H	4.279742	0.358351	-0.010239

Table S8. Atomic coordinates of the optimized structure of [Cu(cyclen)Cl_2].

35			
Cu	0.398149	0.380828	-0.185296
Cl	1.951302	0.320859	-1.972232
N	-0.801533	1.533483	-1.510672
N	-0.775986	-1.358543	-1.204955
Cl	1.839917	-0.259004	1.518451
N	-0.843433	1.296773	1.291035
N	-1.128394	-1.808280	1.822730
C	-1.407077	0.632367	-2.534765
C	-1.881713	-0.693200	-1.926233
C	-1.127977	-2.633984	-0.533035
C	-1.906062	-2.466123	0.782558
C	-1.678328	-0.720051	2.603626
C	-2.030267	0.583411	1.848990
C	-1.741780	2.385273	-0.733902
C	-1.177063	2.611478	0.672824
H	-2.285724	-1.318623	-2.734908
H	-2.700689	-0.519263	-1.225918
H	-2.241695	1.123146	-3.045805
H	-0.628219	0.432623	-3.269155
H	-1.710859	-3.283691	-1.201144
H	-0.190432	-3.149156	-0.317204
H	-2.221673	-3.472346	1.091508
H	-2.832729	-1.911597	0.593724
H	-2.558117	1.251563	2.543205
H	-2.716625	0.361874	1.031735
H	-2.596773	-1.042627	3.107758
H	-0.961741	-0.486740	3.394352
H	-1.893258	3.174474	1.281889
H	-0.257370	3.195413	0.612499
H	-1.919668	3.344521	-1.228843
H	-2.701416	1.872518	-0.674763
H	-0.127674	-1.766629	1.687504
H	-0.054604	2.076959	-1.938500
H	-0.131050	1.395716	2.014558
H	0.020461	-1.493723	-1.827615

Table S9. Atomic coordinates of the optimized structure of [Cu(cyclen{$CH_2CH_2NH_2$}$_2$)]$^{2+}$.

49			
Cu	-0.381445	0.069115	0.148024
N	2.615927	-0.711585	-1.615379
N	-0.988343	1.544822	-1.195077
N	-0.699984	-1.287455	-1.429467
N	1.591081	0.485380	0.921079
N	-1.030391	1.410156	1.633577
N	-1.099494	-1.426247	1.405816
C	-1.411615	0.879492	-2.474034

C	-1.791107	-0.575826	-2.205478
C	-1.254847	-2.538227	-0.776506
C	-2.008277	-2.221966	0.516468
C	-1.714165	-0.796970	2.627789
C	-2.115394	0.658654	2.361419
C	-2.076777	2.277805	-0.460838
C	-1.568031	2.633901	0.934213
H	-1.986630	-1.098220	-3.146028
H	-2.708552	-0.620106	-1.619997
H	-2.252785	1.404938	-2.930442
H	-0.581693	0.944096	-3.174927
H	-1.901329	-3.073936	-1.476359
H	-0.414107	-3.194412	-0.552373
H	-2.324194	-3.151100	0.996607
H	-2.907156	-1.635176	0.329465
H	-2.363477	1.153800	3.304748
H	-3.009892	0.692196	1.739509
H	-2.585901	-1.362281	2.962774
H	-0.979917	-0.852818	3.429613
H	-2.357744	3.101933	1.526263
H	-0.759953	3.360508	0.853726
H	-2.377471	3.179645	-0.998697
H	-2.947503	1.624779	-0.408817
H	-0.329641	-2.026510	1.697308
H	-0.228677	2.195117	-1.390336
C	0.162369	1.737384	2.497274
C	0.420400	-1.665426	-2.386896
C	1.452385	1.770582	1.663895
C	1.800685	-1.946643	-1.779012
H	2.295781	-2.671218	-2.433793
H	1.709567	-2.428176	-0.803681
H	0.084986	-2.547887	-2.939037
H	0.520550	-0.863230	-3.115917
H	2.299002	1.965086	2.324663
H	1.427406	2.584174	0.938679
H	0.008205	2.688860	3.011533
H	0.251545	0.970432	3.265365
H	3.541774	-0.936637	-1.254280
H	1.974780	-0.242958	1.519777
H	2.744334	-0.231468	-2.504434
H	2.156316	0.506021	0.064419