Supplementary Information

Stable astatine-metal bond in gold-based carriers for targeted alpha-particle therapy: role of charge-shift bonding

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Methods

The two-component relativistic density functional theory, which was proven to be accurate for investigating At-containing systems,[1,2] entails replacing the orbital representation by spinors that are complex vector functions of two components (2c). The Generalized Kohn-Sham (GKS) method, implemented in the Gaussian 16 rev. A.03 program,[3] takes advantages of relativistic pseudopotentials containing scalar and spin-dependent terms to treat the electron correlation and the relativistic effects on an equal footing. Among 36 DFT functionals benchmarked on At-containing systems,[2] the PBE0 and PW6B95 hybrid functionals[4,5] clearly emerged among the best performing ones. The small core pseudopotentials ECP*n*MDF were used for the Rh, I, Ir, Au and At atoms,[6–9] in conjunction with the dhf-TZVP basis sets supplemented with two-component extensions,[10] for describing the explicitly treated electrons. Polarized valence triple zeta basis sets, namely def2-TZVP,[11] were also used for the remaining atoms. All basis sets are collectively referred to as TZVP, and were used in both 2c-relativistic calculations and scalar-relativistic (spin-dependent terms omitted in pseudopotentials) calculations. On the basis of previous results (ref. 12), the structure of each complex has been optimized at both 2c-relativistic and scalar-relativistic levels without noticing any modification of the symmetry point groups.

Introduced by Becke and Edgecombe,[13] ELF is a signature of the distribution of electronic pairs and the analysis of its topology is a powerful tool for the characterization of bonding schemes.[14] In the ELF analysis, each basin is assigned to a uniform color according to its synaptic order type:[15] cores (labeled C), monosynaptic or valence non-bonding basins (labeled V) usually corresponding to lone pair regions, while disynaptic (and polysynaptic) or bonding basins (also labeled V for two or more nuclei) characterize the bonding pairs. Furthermore, it is found from experimental and theoretical reports that QTAIM, defined by Bader,[16] can be used to gain insight into the nature of the chemical bonding.[17] The electron

density exhibits large maxima ($\nabla\rho = 0$) at the nuclear positions, and the atomic basins are delimited by zero-flux surfaces of the electron density gradient field. The QTAIM basins being only atomic, integrating the electron density over each basin directly yields its electron population and its corresponding atomic charge, q. Overall, among the saddle points of the gradient field, a bond critical point (BCP) is only connected to two maxima (nuclei) by the trajectories of the gradient field (bond path). Details on the extension of the ELF and QTAIM topological analysis in the framework of 2c-DFT calculations can be found in refs. 18–20, as well as on program files which implement the treatment of 2c wave functions. All the topological analyses were carried out using a modified version of the TopChem2 program.[21,22] The typical command lines for analyzing a WFN file corresponding to a 2c wave function are, for QTAIM:

>topchem2 wfn:2c_file.wfn level:so notimer function:rho pop:cov cp:y refine:f proc:24

and for ELF:

>topchem2 wfn:2c_file.wfn level:so notimer function:elf pop:cov refine:f proc:24

The visualization of the interatomic surface gradient paths (Fig. 2) was carried out using mpi-TopMod (https://www.lct.jussieu.fr/pagesperso/fuster/topmod.html). All pictures were obtained using the VMD software.[23]

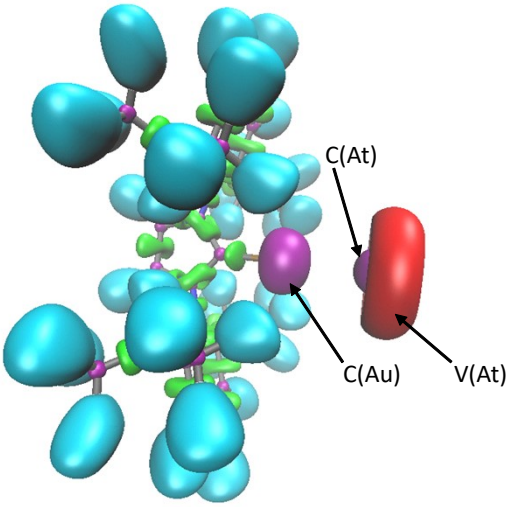

Fig. S1 ELF localization domains of **1a**, disclosing the basins related to the Au–At bond. Color code: magenta for core basins, red for the valence nonbonding basins, green for the valence bonding basins, cyan for the protonated bonding basins.

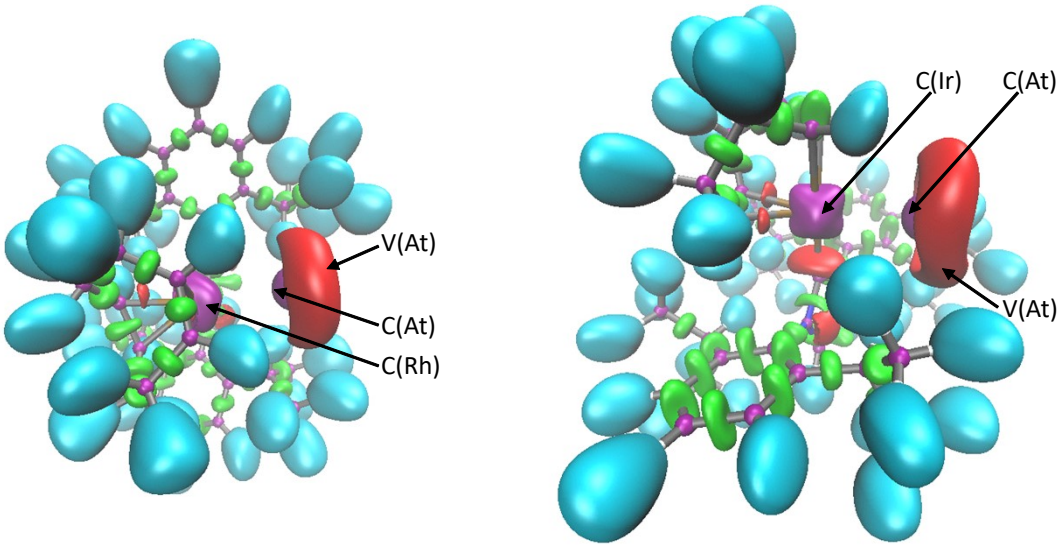

Fig. S2 ELF localization domains of **2a** (left) and **3a** (right), disclosing the basins related to the M–At (M = Rh, Ir) bonds. Color code: magenta for core basins, red for the valence nonbonding basins, green for the valence bonding basins, cyan for the protonated bonding basins.

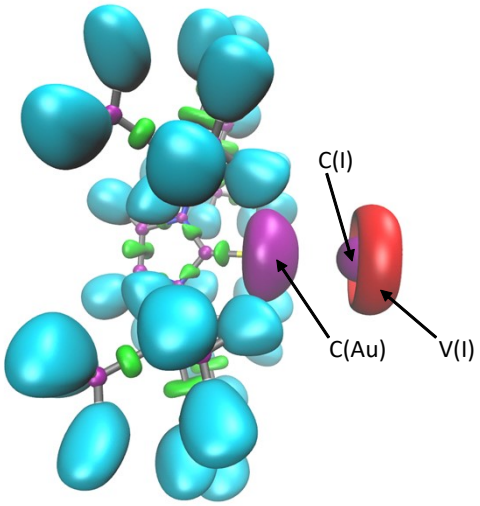

Fig. S3 ELF localization domains of **1a**, disclosing the basins related to the Au–I bond. Color code: magenta for core basins, red for the valence nonbonding basins, green for the valence bonding basins, cyan for the protonated bonding basins.

Table S1. Metal-halide bond snapping energies (BSE) in **1a**-**3a** complexes and coefficients of determination (R^2) for linear correlations with selected QTAIM descriptors.

complex	BSE[12] (kJ/mol)	ΔG_R [a] (kJ/mol)	δ (a.u)	δ_π (%)	q(M) (a.u)	q(At) (a.u)	Δq (a.u)
1a	562.7	0.0	1.16	23.0	-0.02	-0.32	0.30
2a	439.0	-145.3	0.75	14.1	+0.34	-0.45	0.79
3a	471.2	-124.8	0.85	15.9	+0.41	-0.35	0.76
R^2		0.985	1.000	0.996	0.844	0.708	0.961

[a] Relative value of the free energy of M–At bond heterolytic dissociation (Scheme 2) in aqueous solution. The Au-At bond in **1a** is taken as reference, T = 298.15 K, $C°$ = 1 mol/L.[12]

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Cartesian coordinates (Å) for the studied complexes

1a

Au	0.00016	0.72184	0.00020
C	-0.00045	-1.27680	-0.00036
N	-1.07040	-2.10485	-0.00051
C	-0.67569	-3.42451	-0.00093
H	-1.38607	-4.23319	-0.00110
C	0.67380	-3.42483	-0.00105
H	1.38380	-4.23384	-0.00136
N	1.06912	-2.10535	-0.00070
C	2.43823	-1.67958	-0.00072
C	3.07949	-1.48981	1.22722
C	4.41465	-1.10212	1.19798
H	4.94072	-0.93969	2.13180
C	5.07730	-0.91100	-0.00077
H	6.11720	-0.60444	-0.00080
C	4.41414	-1.10055	-1.19949
H	4.93981	-0.93688	-2.13333
C	3.07898	-1.48825	-1.22868
C	2.37747	-1.66938	2.55502
H	1.35064	-1.98492	2.35617
C	2.37637	-1.66603	-2.55641
H	1.35001	-1.98311	-2.35756
C	3.03741	-2.76085	3.39504
H	3.06456	-3.71564	2.86437
H	2.48734	-2.90568	4.32824
H	4.06532	-2.49597	3.65529
C	2.30615	-0.34919	3.32015
H	1.74991	-0.48104	4.25188
H	1.80946	0.42385	2.73013
H	3.30476	0.01323	3.57769
C	3.03695	-2.75509	-3.39904
H	3.06565	-3.71087	-2.87023
H	4.06432	-2.48851	-3.65966
H	2.48629	-2.89876	-4.33207
C	2.30314	-0.34435	-3.31879
H	1.74670	-0.47493	-4.25058
H	3.30124	0.01980	-3.57592
H	1.80575	0.42686	-2.72695
C	-2.43933	-1.67848	-0.00026
C	-3.08035	-1.48730	-1.22811
C	-3.08010	-1.48789	1.22780
C	-4.41533	-1.09899	-1.19866
C	-4.41508	-1.09956	1.19881
C	-5.07802	-0.90864	0.00019
H	-4.94121	-0.93543	-2.13240
H	-4.94077	-0.93645	2.13273
H	-6.11777	-0.60159	0.00037
C	-2.37764	-1.66699	2.55543
C	-3.03870	-2.75643	3.39719
C	-2.30392	-0.34593	3.31883
H	-1.35140	-1.98433	2.35639
H	-3.06774	-3.71180	2.86765
H	-2.48817	-2.90103	4.33015
H	-4.06599	-2.48965	3.65793
H	-1.80621	0.42554	2.72759
H	-3.30188	0.01841	3.57621
H	-1.74755	-0.47744	4.25053
C	-2.37816	-1.66577	-2.55596
C	-2.30456	-0.34434	-3.31874
C	-3.03941	-2.75478	-3.39812
H	-1.35188	-1.98323	-2.35729
H	-1.80668	0.42682	-2.72724
H	-1.74841	-0.47541	-4.25063
H	-3.30256	0.02017	-3.57571
H	-3.06838	-3.71040	-2.86904
H	-4.06674	-2.48785	-3.65855
H	-2.48906	-2.89895	-4.33125
At	0.00103	3.37385	0.00099

2a

Rh	-0.06150	-0.32727	1.24345
C	-0.28280	0.57217	-0.60686
N	0.65539	1.31127	-1.28094
C	0.21971	1.64499	-2.54637
C	-1.00695	1.12169	-2.69071
N	-1.31072	0.48545	-1.50359
C	-1.00640	1.19742	2.41289
C	-1.93822	0.22469	2.01318
C	-2.51066	-0.86200	2.88024
C	-1.45635	-1.55096	3.74774
C	-0.12908	-1.63381	3.03876
C	0.89553	-0.71537	3.15951
C	0.86122	0.54652	3.97412
C	-0.45019	1.31703	3.81613
H	-1.01391	2.12385	1.85024
H	-2.58218	0.47941	1.17968
H	0.81895	2.23150	-3.21868
H	-1.69589	1.14314	-3.51663
H	-2.96795	-1.60133	2.21636
H	-3.32748	-0.46491	3.50026
H	-1.79238	-2.56202	3.99133
H	-1.34083	-1.03488	4.70318
H	0.13753	-2.60744	2.64071
H	1.88752	-1.05108	2.86737
H	1.68819	1.17798	3.63701
H	1.06024	0.32250	5.03162
H	-1.19255	0.97354	4.54057

H	-0.27941	2.37116	4.05031
C	-2.64122	-0.01559	-1.28997
C	-2.91109	-1.37771	-1.46235
C	-3.65103	0.91739	-1.00662
C	-4.22539	-1.80032	-1.28319
C	-4.94816	0.44082	-0.84999
C	-5.23382	-0.90611	-0.97542
H	-4.46123	-2.85118	-1.39762
H	-5.74663	1.13787	-0.62328
C	1.90373	1.82300	-0.77710
C	1.86858	2.96053	0.04533
C	3.11530	1.26485	-1.21236
C	3.07404	3.45193	0.53247
C	4.29181	1.80364	-0.69769
C	4.27660	2.86697	0.18266
H	3.07182	4.31678	1.18424
H	5.24010	1.37551	-0.99737
H	-6.25030	-1.25951	-0.84247
H	5.20717	3.25835	0.57841
C	-1.85121	-2.35701	-1.90599
C	-1.87639	-2.50622	-3.42816
C	-1.97035	-3.71801	-1.23281
H	-0.87693	-1.95234	-1.62351
H	-1.72682	-1.54851	-3.93227
H	-1.08184	-3.18310	-3.75205
H	-2.83232	-2.91753	-3.76585
H	-1.99482	-3.62134	-0.14582
H	-2.86160	-4.26326	-1.55639
H	-1.10059	-4.32693	-1.48716
C	3.20899	0.18321	-2.26828
C	4.31192	-0.83440	-1.99034
C	3.44905	0.80336	-3.64844
H	2.26034	-0.35881	-2.28248
H	4.25017	-1.22562	-0.97494
H	4.21310	-1.67689	-2.67862
H	5.30578	-0.40516	-2.14537
H	2.66790	1.50632	-3.94045
H	4.40028	1.34274	-3.66557
H	3.49388	0.01952	-4.40902
C	-3.39250	2.40759	-0.89846
C	-3.96505	3.01856	0.37872
C	-3.94477	3.13944	-2.12258
H	-2.31155	2.56415	-0.87919
H	-3.58594	2.51994	1.27209
H	-3.69348	4.07576	0.43857
H	-5.05618	2.96346	0.39809
H	-3.51992	2.75522	-3.05184
H	-5.03069	3.02807	-2.18326
H	-3.71926	4.20741	-2.06349
C	0.59200	3.73028	0.30644
C	0.39587	4.79904	-0.77231
C	0.53922	4.37436	1.68680
H	-0.24084	3.02919	0.23342
H	0.35329	4.36410	-1.77239
H	-0.53546	5.34678	-0.60273
H	1.21908	5.51844	-0.75324
H	0.78578	3.66158	2.47489
H	1.22947	5.21804	1.76561
H	-0.46349	4.76393	1.87953
At	1.52559	-2.29089	0.05071

3a

Ir	-0.07025	-0.34902	1.12925
C	-0.27908	0.62130	-0.67661
N	0.65833	1.39443	-1.31679
C	0.21703	1.78789	-2.56282
C	-1.00687	1.26681	-2.73134
N	-1.30879	0.57252	-1.57690
C	-1.01673	1.13276	2.32854
C	-1.95484	0.15770	1.88806
C	-2.54764	-0.92772	2.74618
C	-1.49188	-1.65859	3.57688
C	-0.16441	-1.70454	2.85847
C	0.86204	-0.77465	3.03184
C	0.79934	0.43578	3.92241
C	-0.50618	1.21296	3.75501
H	-1.06081	2.09110	1.82204
H	-2.61980	0.45542	1.08504
H	0.81212	2.41103	-3.20505
H	-1.69657	1.32422	-3.55479
H	-3.03611	-1.64083	2.07571
H	-3.34075	-0.51963	3.38875
H	-1.82521	-2.68054	3.77338
H	-1.37302	-1.18889	4.55606
H	0.12939	-2.67911	2.48145
H	1.86825	-1.11261	2.79491
H	1.63932	1.08371	3.65573
H	0.95579	0.14588	4.97075
H	-1.26983	0.84551	4.44520
H	-0.34498	2.25924	4.02730
C	-2.63562	0.04870	-1.39728
C	-2.88698	-1.30833	-1.62665
C	-3.65983	0.95887	-1.09258
C	-4.19919	-1.75164	-1.48724
C	-4.95394	0.46272	-0.97779
C	-5.22262	-0.88086	-1.16249
H	-4.42135	-2.79958	-1.64690
H	-5.76362	1.14152	-0.73596
C	1.91099	1.88221	-0.79965
C	1.88560	2.98574	0.06754
C	3.11735	1.34015	-1.26882

C	3.09678	3.45649	0.56076
C	4.29986	1.85661	-0.74555
C	4.29490	2.88488	0.17577
H	3.10219	4.29462	1.24656
H	5.24458	1.43972	-1.07129
H	-6.23724	-1.24981	-1.06153
H	5.22995	3.25956	0.57705
C	-1.80941	-2.25970	-2.08878
C	-1.81576	-2.36140	-3.61503
C	-1.91899	-3.64194	-1.45827
H	-0.84385	-1.85170	-1.78307
H	-1.67343	-1.38624	-4.08686
H	-1.00931	-3.01785	-3.95144
H	-2.76258	-2.77368	-3.97616
H	-1.95623	-3.57802	-0.36924
H	-2.80061	-4.18682	-1.80754
H	-1.04035	-4.23384	-1.72244
C	3.19761	0.29913	-2.36596
C	4.30407	-0.72778	-2.14057
C	3.42096	0.96920	-3.72545
H	2.24803	-0.24112	-2.38887
H	4.26087	-1.15234	-1.13774
H	4.19424	-1.54643	-2.85548
H	5.29526	-0.29317	-2.29720
H	2.63487	1.67965	-3.98353
H	4.37068	1.51140	-3.73297
H	3.45958	0.21348	-4.51434
C	-3.41933	2.44557	-0.91494
C	-4.01539	2.99184	0.38079
C	-3.96411	3.22658	-2.11172
H	-2.34049	2.61279	-0.87342
H	-3.64147	2.45780	1.25564
H	-3.75705	4.04822	0.49160
H	-5.10593	2.92347	0.38315
H	-3.52357	2.89008	-3.05213
H	-5.04786	3.10674	-2.19161
H	-3.75136	4.29304	-2.00098
C	0.61269	3.74372	0.37473
C	0.41415	4.86769	-0.64577
C	0.56937	4.31285	1.78778
H	-0.22224	3.04939	0.27038
H	0.36623	4.48569	-1.66715
H	-0.51532	5.40740	-0.44349
H	1.23874	5.58387	-0.59334
H	0.81472	3.55606	2.53388
H	1.26470	5.14730	1.90912
H	-0.43040	4.69658	2.00586
At	1.56518	-2.25038	-0.08115

1b

Au	-0.00006	-0.00004	1.47136
C	0.00005	0.00002	-0.50405
N	1.07011	0.00005	-1.33322
C	0.67466	0.00008	-2.65266
H	1.38491	0.00011	-3.46137
C	-0.67460	0.00007	-2.65265
H	-1.38487	0.00008	-3.46135
N	-1.07002	0.00003	-1.33320
C	-2.43900	0.00000	-0.90751
C	-3.08018	1.22788	-0.71688
C	-4.41515	1.19868	-0.32848
H	-4.94099	2.13250	-0.16522
C	-5.07792	-0.00005	-0.13768
H	-6.11765	-0.00008	0.16945
C	-4.41509	-1.19877	-0.32845
H	-4.94089	-2.13260	-0.16518
C	-3.08013	-1.22790	-0.71686
C	-2.37747	2.55554	-0.89465
H	-1.35333	2.35673	-1.21890
C	-2.37735	-2.55554	-0.89460
H	-1.35328	-2.35669	-1.21903
C	-3.04349	3.40317	-1.97642
H	-3.07943	2.87768	-2.93376
H	-2.49182	4.33554	-2.12047
H	-4.06853	3.66522	-1.70242
C	-2.29542	3.31268	0.42957
H	-1.73955	4.24485	0.29930
H	-1.79337	2.71748	1.19504
H	-3.29117	3.56839	0.80106
C	-3.04347	-3.40336	-1.97615
H	-3.07963	-2.87798	-2.93355
H	-4.06843	-3.66549	-1.70195
H	-2.49172	-4.33568	-2.12018
C	-2.29503	-3.31249	0.42972
H	-1.73914	-4.24466	0.29948
H	-3.29070	-3.56819	0.80141
H	-1.79287	-2.71716	1.19501
C	2.43912	0.00005	-0.90760
C	3.08028	-1.22784	-0.71700
C	3.08026	1.22794	-0.71694
C	4.41526	-1.19868	-0.32867
C	4.41524	1.19877	-0.32861
C	5.07807	0.00005	-0.13791
H	4.94110	-2.13250	-0.16545
H	4.94106	2.13260	-0.16533
H	6.11782	0.00005	0.16916
C	2.37746	2.55558	-0.89453
C	3.04349	3.40349	-1.97606
C	2.29522	3.31243	0.42985

H	1.35336	2.35674	-1.21890
H	3.07959	2.87818	-2.93350
H	2.49173	4.33582	-2.11999
H	4.06847	3.66561	-1.70192
H	1.79311	2.71704	1.19513
H	3.29092	3.56811	0.80149
H	1.73932	4.24461	0.29972
C	2.37750	-2.55549	-0.89467
C	2.29528	-3.31242	0.42966
C	3.04354	-3.40332	-1.97626
H	1.35340	-2.35665	-1.21903
H	1.79317	-2.71708	1.19498
H	1.73940	-4.24460	0.29948
H	3.29099	-3.56810	0.80129
H	3.07962	-2.87795	-2.93367
H	4.06853	-3.66543	-1.70213
H	2.49180	-4.33565	-2.12024
Cl	-0.00022	-0.00010	3.73340

1c

Au	-0.00009	1.04743	-0.00081
C	0.00018	-0.94811	0.00077
N	1.07003	-1.77596	0.00135
C	0.67509	-3.09540	0.00244
H	1.38542	-3.90408	0.00304
C	-0.67446	-3.09548	0.00254
H	-1.38469	-3.90426	0.00326
N	-1.06957	-1.77610	0.00151
C	-2.43859	-1.34962	0.00126
C	-3.07949	-1.15988	-1.22688
C	-4.41427	-0.77087	-1.19783
H	-4.94014	-0.60828	-2.13172
C	-5.07675	-0.57856	0.00081
H	-6.11630	-0.27084	0.00064
C	-4.41390	-0.76824	1.19967
H	-4.93949	-0.60359	2.13337
C	-3.07912	-1.15723	1.22918
C	-2.37763	-1.34073	-2.55460
H	-1.35113	-1.65744	-2.35575
C	-2.37684	-1.33513	2.55707
H	-1.35074	-1.65336	2.35863
C	-3.03878	-2.43182	-3.39417
H	-3.06704	-3.38637	-2.86312
H	-2.48887	-2.57764	-4.32730
H	-4.06636	-2.16586	-3.65456
C	-2.30498	-0.02098	-3.32040
H	-1.74881	-0.15382	-4.25201
H	-1.80784	0.75219	-2.73102
H	-3.30321	0.34223	-3.57823
C	-3.03858	-2.42327	3.39999
H	-3.06814	-3.37921	2.87153
H	-4.06572	-2.15559	3.66035
H	-2.48820	-2.56713	4.33314
C	-2.30261	-0.01330	3.31912
H	-1.74635	-0.14406	4.25097
H	-3.30041	0.35166	3.57613
H	-1.80482	0.75768	2.72741
C	2.43902	-1.34936	0.00089
C	3.07983	-1.15726	1.22871
C	3.07957	-1.15913	-1.22736
C	4.41456	-0.76812	1.19899
C	4.41431	-0.76995	-1.19852
C	5.07707	-0.57797	0.00002
H	4.94036	-0.60370	2.13260
H	4.93991	-0.60695	-2.13249
H	6.11658	-0.27013	-0.00032
C	2.37731	-1.33942	-2.55494
C	3.03908	-2.42904	-3.39592
C	2.30306	-0.01894	-3.31934
H	1.35120	-1.65731	-2.35594
H	3.06862	-3.38405	-2.86578
H	2.48874	-2.57453	-4.32884
H	4.06623	-2.16181	-3.65671
H	1.80529	0.75309	-2.72898
H	3.30084	0.34556	-3.57705
H	1.74675	-0.15137	-4.25093
C	2.37785	-1.33554	2.55671
C	2.30368	-0.01389	3.31909
C	3.03985	-2.42383	3.39923
H	1.35172	-1.65379	2.35841
H	1.80570	0.75719	2.72766
H	1.74763	-0.14492	4.25102
H	3.30151	0.35109	3.57597
H	3.06936	-3.37965	2.87054
H	4.06702	-2.15614	3.65943
H	2.48968	-2.56794	4.33247
I	-0.00051	3.60636	-0.00285