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Electronic Supplementary Information

# Polarised Covalent Thorium(IV)- and

# Uranium(IV)-Silicon Bonds

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### **1. General Procedures**

All manipulations were conducted under argon with the strict exclusion of oxygen and water by using Schlenk line and glove box techniques. THF, Et<sub>2</sub>O, toluene and pentane were purged with ultra-high-purity grade argon (Airgas) and passed through columns containing alumina catalyst and molecular sieves before use. Hexane was dried by refluxing over potassium and stored over a potassium mirror, then degassed before use. For NMR spectroscopy, C<sub>6</sub>D<sub>6</sub> was dried by refluxing over K, and was vacuum transferred and degassed by three freeze-pump-thaw cycles before use. NMR spectra were recorded on either a Bruker AVIII HD 400 spectrometer operating at 400.07 (<sup>1</sup>H), 100.60 ( ${}^{13}C{}^{1}H{}$ ) or 79.48 ( ${}^{29}Si{}^{1}H{}$ ) MHz, or a Bruker AVIII HD 500 spectrometer operating at 500.19 (<sup>1</sup>H), 125.77 (<sup>13</sup>C{<sup>1</sup>H}), 99.37 (<sup>29</sup>Si{<sup>1</sup>H}). NMR spectra were referenced to TMS. FTIR spectra were recorded on a Bruker Alpha spectrometer with Platinum-ATR module. UV-Vis-NIR spectroscopy were recorded on a Perkin Elmer Lambda 750 spectrometer. Data was collected in a 1mm path length cuvette loaded in an MBraun UniLab glovebox and was run versus toluene reference solvent. Elemental analysis was carried out by Mr Martin Jennings and Mrs Anne Davies at the Microanalytical service, Department of Chemistry, the University of Manchester. KCp',<sup>1</sup>  $KSi(SiMe_3)_{3,2}$  [U(Cp')<sub>3</sub>Cl] (1-U),<sup>3</sup> and [ThCl<sub>4</sub>(DME)<sub>2</sub>]<sup>4</sup> were synthesised according to literature procedures.  $[Th(Cp')_3Cl]$  (1-Th)<sup>5</sup> was synthesised by modification of literature procedures. Caution: Natural abundance thorium and uranium are weak  $\alpha$ -emitters, thus we recommend the use of suitable designated radiochemical laboratories with  $\alpha$ -counting equipment available for safe manipulation of compounds containing these elements.

#### 2. Experimental Details: 1-Th, 2-An

**Modified preparation of [Th(Cp')<sub>3</sub>Cl] (1-Th) from literature procedures.**<sup>5</sup> To a precooled (-78 °C) suspension of [ThCl<sub>4</sub>(DME)<sub>2</sub>] (2.7704 g, 5 mmol) in THF (40 mL), a solution of KCp' (2.6897 g, 15.25 mmol) in Et<sub>2</sub>O (20 mL) was added dropwise. The resulting yellow suspension was warmed to room temperature and stirred for 18 hours. All volatiles were subsequently removed *in vacuo*, and the beige solid was extracted with hot hexane (100 mL, 60 °C). Upon cooling colourless needles of **1-Th** formed which were isolated at room temperature. Further crops of **1-Th** were obtained on storage of the mother liquor at -25 °C. Yield = 2.4420 g, 3.59 mmol, 72 %. All analytical data is consistent with literature values.<sup>5</sup> <sup>29</sup>Si {<sup>1</sup>H} NMR (79.48 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K):  $\delta$  = -8.46 (Cp-*Si*(CH<sub>3</sub>)<sub>3</sub>).

**Preparation of [Th(Cp')<sub>3</sub>{Si(SiMe<sub>3</sub>)<sub>3</sub>}] (2-Th).** To a pre-cooled (-78 °C) solution of [Th(Cp')<sub>3</sub>Cl] (0.6793 g, 1 mmol) in toluene (20 mL) was added KSi(SiMe<sub>3</sub>)<sub>3</sub> (0.2868 g, 1 mmol) in toluene (20 mL) dropwise. The yellow solution was warmed to room temperature and stirred for one hour. All volatiles were subsequently removed *in vacuo*, and the off-white solid was extracted with pentane (30 mL). The resulting solution was concentrated to 5 mL and storage at -25 °C led to the formation of **2-Th** as colourless plates. Yield = 0.6627 g, 0.74 mmol, 74 %. Anal. Calcd for C<sub>33</sub>H<sub>66</sub>Si<sub>7</sub>Th: C, 44.46; H, 7.46. Found: C, 43.37; H, 7.45. Low carbon values are reproducibly obtained for silicon-rich organometallic complexes due to the formation of silicon carbides.<sup>6</sup> <sup>1</sup>H NMR (400.07 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K): δ = 0.34 (s, 27H, Cp-Si(CH<sub>3</sub>)<sub>3</sub>), 0.66 (s, 27H, Si {Si(CH<sub>3</sub>)<sub>3</sub>}<sub>3</sub>), 6.26 (s, br, 6H, Cp-H), 6.72 (s, br, 6H, Cp-H). <sup>13</sup>C {<sup>1</sup>H} NMR (100.60 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K): δ = 1.18 (Cp-Si(CH<sub>3</sub>)<sub>3</sub>), 7.01 (Si {Si(CH<sub>3</sub>)<sub>3</sub>}<sub>3</sub>), 119.78 (Cp-CH), 121.61 (Cp-CH), 131.01 (Cp-C). <sup>29</sup>Si {<sup>1</sup>H} NMR (79.48 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K): δ = -108.92 (*Si*Th), -7.87 (Cp-*Si*(CH<sub>3</sub>)<sub>3</sub>), -2.18 (Si {*Si*(CH<sub>3</sub>)<sub>3</sub>}<sub>3</sub>). FTIR v/ cm<sup>-1</sup>: 2950 (m), 2890 (w), 1405 (w), 1365 (w), 1248 (m), 1171 (m), 1044 (m), 904 (m), 818 (s), 777 (s), 749 (s).

Preparation of [U(Cp')<sub>3</sub>{Si(SiMe<sub>3</sub>)<sub>3</sub>}] (2-U). To a pre-cooled (-78 °C) solution of [U(Cp')<sub>3</sub>Cl] (0.6853 g, 1 mmol) in toluene (20 mL) was added KSi(SiMe<sub>3</sub>)<sub>3</sub> (0.2868 g, 1 mmol) in toluene (20 mL) dropwise. The resultant dark green solution was warmed to room temperature and stirred for one hour. All volatiles were subsequently removed in vacuo, and the dark green solid was extracted with pentane (40 mL). The resulting solution was concentrated to 5 mL and storage at -25 °C led to the formation of 2-U as green plates. Yield = 0.5777 g, 0.64 mmol, 64 %. Anal. Calcd for C<sub>33</sub>H<sub>66</sub>Si<sub>7</sub>U: C, 44.16; H, 7.41. Found: C, 43.52; H, 7.40. Low carbon values are reproducibly obtained for silicon-rich organometallic complexes due to the formation of silicon carbides.<sup>6</sup> <sup>1</sup>H NMR (400.07 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K): δ = -6.67 (s, 27H, Si{Si(CH<sub>3</sub>)<sub>3</sub>}), -5.62 (s, 27H, Cp-Si(CH<sub>3</sub>)<sub>3</sub>), 0.25 (s, br, 6H, Cp-H), 0.37 (s, br, 6H, Cp-H). <sup>13</sup>C{<sup>1</sup>H} NMR (100.60 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K):  $\delta = 1.66$  (Cp-Si(CH<sub>3</sub>)<sub>3</sub>), 10.60  $(Si{Si(CH_3)_3})$ . Resonances derived from Cp-C and Cp-CH could not be observed. <sup>29</sup>Si{<sup>1</sup>H} NMR (79.48 MHz,  $C_6D_6$ , 298 K):  $\delta = -137.09$  (USi), -101.59 (Cp-Si(CH<sub>3</sub>)<sub>3</sub>), -137.09 $(Si \{Si(CH_3)_3\}_3)$ . Evans Method (C<sub>6</sub>D<sub>6</sub>, 298 K) 2.92 µ<sub>B</sub>. ATR-IR v/ cm<sup>-1</sup>: 2950 (m), 2895 (m), 1438 (w), 1405 (m), 1369 (w), 1248 (m), 1171 (m), 1042 (m), 902 (m), 820 (s), 781 (s), 751 (s), 620 (s).

## 3. NMR Spectra: 2-An



Figure S1. <sup>1</sup>H NMR spectrum (400.07 MHz) of 2-Th in  $C_6D_6$ . \* denotes residual pentane.



Figure S2. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (100.60 MHz) of 2-Th in  $C_6D_6$ . \* denotes residual pentane.



Figure S3. <sup>29</sup>Si{<sup>1</sup>H} NMR spectrum (79.480 MHz) of 2-Th in  $C_6D_6$ .



Figure S4.  $^{1}H-^{13}C$  HSQC NMR spectrum of 2-Th in C<sub>6</sub>D<sub>6</sub>.



Figure S5. <sup>1</sup>H–<sup>13</sup>C HMBC NMR spectrum of 2-Th in C<sub>6</sub>D<sub>6</sub>.



Figure S6.  $^{1}H-^{29}Si$  HMBC NMR spectrum of 2-Th in C<sub>6</sub>D<sub>6</sub>.



Figure S7. <sup>1</sup>H NMR spectrum (400.07 MHz) of 2-U in C<sub>6</sub>D<sub>6</sub>. \* denotes residual pentane.



Figure S8. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (100.60 MHz) of **2-U** in  $C_6D_6$ . \* denotes residual pentane.



**Figure S9.** <sup>29</sup>Si{<sup>1</sup>H} NMR spectrum (79.48 MHz) of **2-U** in C<sub>6</sub>D<sub>6</sub>. \* denotes silicone grease impurity.



Si(SiMe<sub>3</sub>)<sub>4</sub>; **2-U**; and, Si(SiMe<sub>3</sub>)<sub>4</sub>, to validate the assignment of **2-U**. Inset shows zoomed in region to better depict the differences in signals between **2-U** and Si(SiMe<sub>3</sub>)<sub>4</sub>.



**Figure S11.** Stacked <sup>29</sup>Si{<sup>1</sup>H} NMR spectra (99.37 MHz) in C<sub>6</sub>D<sub>6</sub> of: **2-U** with one equivalent of Si(SiMe<sub>3</sub>)<sub>4</sub>; **2-U**; and, Si(SiMe<sub>3</sub>)<sub>4</sub>, to validate the assignment of **2-U**. Insets show zoomed in regions to better depict the differences in signals between **2-U** and Si(SiMe<sub>3</sub>)<sub>4</sub>.



Figure S12. Stacked <sup>1</sup>H NMR spectra (500.19 MHz) in  $C_6D_6$  of: 2-U with silicone grease; and, 2-U, to highlight the presence of silicone grease impurity in 2-U. Inset shows zoomed in region to better depict the change in intensities.



Figure S13. Stacked <sup>29</sup>Si{<sup>1</sup>H} NMR spectra (99.37 MHz) in  $C_6D_6$  of: 2-U with silicone grease; and, 2-U, to highlight the presence of silicone grease impurity in 2-U with a decrease in intensity of all other signals.



**Figure S14.** <sup>1</sup>H NMR spectrum (400.07 MHz) of **2-U** in  $C_6D_6$  with a glass capillary containing 1:1  $C_6H_6$ :  $C_6D_6$  used to determine the magnetic susceptibility in solution at 298 K.



Figure S15. ATIR spectra of 2-Th between 398–4000 cm<sup>-1</sup>.



Figure S16. ATIR spectra of 2-U between 398–4000 cm<sup>-1</sup>.

## 5. UV-Vis-NIR Spectra: 2-An



**Figure S17.** UV-Vis-NIR spectra of **2-U** in toluene (25 mM) between 6000–27000 cm<sup>-1</sup> (1667– 370 nm), inset shows zoomed in region between 6000–17000 cm<sup>-1</sup> (1667–588 nm).

## 6. SQUID: 1-U, 2-U

Static variable-temperature magnetic moment data were recorded in an applied DC field of 0.5 T on a Quantum Design MPMS XL7 superconducting quantum interference device (SQUID) using doubly recrystallised powdered samples. Samples were carefully checked for purity and data reproducibility between several independently prepared batches for each compound examined. Care was taken to ensure complete thermalisation of the sample before each data point was measured, and samples were immobilised in an eicosane matrix to prevent sample reorientation during measurements. Diamagnetic corrections were applied using tabulated Pascal constants and measurements were corrected for the effect of the blank sample holders (flame sealed Wilmad NMR tube and straw) and eicosane matrix.



**Figure S18.** Variable-temperature SQUID magnetometry plot of  $\mu_{eff}$  vs T for 1-U (red) and 2-U (blue) over the temperature range 2–300 K. Line is a guide to the eye only.



**Figure S19.** Variable-temperature SQUID magnetometry plot of  $\chi T$  vs T for 1-U (red) and 2-U (blue) over the temperature range 2–300 K. Line is a guide to the eye only.



**Figure S20.** Variable-temperature SQUID magnetic data for powdered **1-U** in a 0.5 T applied magnetic field, presented as: Top Left –  $\mu_{eff}$  vs T; Top Right –  $\chi$ T vs T; Bottom Left –  $\chi$  vs T; Bottom Right –  $\chi^{-1}$  vs T.



**Figure S21.** Variable-temperature SQUID magnetic data for powdered **2-U** in a 0.5 T applied magnetic field, presented as: Top Left –  $\mu_{eff}$  vs T; Top Right –  $\chi$ T vs T; Bottom Left –  $\chi$  vs T; Bottom Right –  $\chi^{-1}$  vs T.

#### 7. General Crystallographic Methods

The crystal data for 1-Th, 2-Th. $(C_5H_{12})_{0.5}$  and 2-U. $(C_5H_{12})_{0.5}$  are compiled in Table S1. Crystals of 1-Th were examined using an Agilent Supernova diffractometer, equipped with an Eos CCD area detector and a Microfocus source with Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å). Crystals of 2-Th.(C<sub>5</sub>H<sub>12</sub>)<sub>0.5</sub> and 2-U.(C<sub>5</sub>H<sub>12</sub>)<sub>0.5</sub> were examined using a Rigaku FR-X diffractometer, equipped with a HyPix 6000HE photon counting pixel array detector with mirror-monochromated Mo K $\alpha$  ( $\lambda = 0.71073$  Å) or Cu K $\alpha$  ( $\lambda = 1.5418$  Å) radiation. Intensities were integrated from data recorded on 0.5° (2-Th.(C<sub>5</sub>H<sub>12</sub>)<sub>0.5</sub>) or 1° (2-U.(C<sub>5</sub>H<sub>12</sub>)<sub>0.5</sub>, 1-Th) frames by  $\omega$  rotation. Cell parameters were refined from the observed positions of all strong reflections in each data set. A Gaussian grid face-indexed with a beam profile was applied for all structures.<sup>7</sup> The structures were solved using SHELXT;<sup>8</sup> the datasets were refined by fullmatrix least-squares on all unique  $F^2$  values,<sup>8</sup> with anisotropic displacement parameters for all non-hydrogen atoms, and with constrained riding hydrogen geometries;  $U_{iso}(H)$  was set at 1.2 (1.5 for methyl groups) times  $U_{eq}$  of the parent atom. The largest features in final difference syntheses were close to heavy atoms and were of no chemical significance. CrysAlisPro<sup>7</sup> was used for control and integration, and SHELX<sup>8,9</sup> was employed through OLEX2<sup>10</sup> for structure solution and refinement. ORTEP-3<sup>11</sup> and POV-Ray<sup>12</sup> were employed for molecular graphics. CCDC 2019267-2019269 contain the supplementary crystal data for this article. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

# 8. Crystallographic Data

	1-Th	2-Th.(C <sub>5</sub> H <sub>12</sub> ) <sub>0.5</sub>	2-U.(C <sub>5</sub> H <sub>12</sub> ) <sub>0.5</sub>
Formula	$C_{27}H_{46}ClSi_{3}Th$	$C_{35.5}H_{72}Si_{7}Th$	$C_{35.5}H_{72}Si_7Th$
Fw	722.40	927.60	933.59
crystal size, mm	0.311 x 0.233 x 0.188	0.261 x 0.09 x 0.035	0.112 x 0.081 x 0.02
crystal system	Trigonal	monoclinic	monoclinic
space group	рЗ	$P2_1/n$	$P2_1/n$
a, Å	15.6676(5)	9.7657(3)	9.78080(10)
b, Å	15.6676(5)	13.0764(3)	13.0503(2)
c, Å	6.8826(2)	36.6701(11)	36.5075(4)
α, °	90	90	90
β, °	90	97.145(3)	97.1250(1)
γ, °	120	90	90
V, Å <sup>3</sup>	1463.15(10)	4646.4(2)	4623.92(10)
Z	1.99998	4	4
$\rho_{calcd, g cm}^{-3}$	1.640	1.326	1.341
μ, mm <sup>-1</sup>	5.324	3.411	11.767
no. of reflections made	3885	61544	68389
no. of unique reflns $R_{int}$	2499, 0.0271	12200, 0.0452	9599, 0.0472
no. of reflns with $F^2 > 2\sigma(F^2)$	2264	10366	8878
transmn coeff range	0.317-0.641	0.457-1.000	0.926-1.000
R, $R_w^a$ (F <sup>2</sup> > 2 $\sigma$ (F <sup>2</sup> ))	0.0279, 0.0492	0.0304, 0.0600	0.0245, 0.0627
R, R <sub>w</sub> <sup>a</sup> (all data)	0.0329, 0.0507	0.0397, 0.0621	0.0269, 0.0640
S <sup>a</sup>	1.022	1.071	1.068
Parameters	91, 0	435, 28	435, 28
max., min. diff map, e Å <sup>-3</sup>	0.595, -0.785	1.802, -1.120	1.053, -1.103

Table S1. Crystallographic Data for 1-Th, 2-Th and 2-U

 $\overline{{}^{a} \text{ Conventional } R = \Sigma ||F_{o}| - |F_{c}||/\Sigma |F_{o}|; R_{w} = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2}/\Sigma w (F_{o}^{2})^{2}]^{1/2}; S = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2}/no. data - no. params)]^{1/2} \text{ for all data.}$ 

## 9. Molecular Structures



**Figure S22.** Solid-state molecular structure of **1-Th** measured at 150 K. Ellipsoids set at 50 % probability; hydrogen atoms and lattice solvent removed for clarity. Selected bond lengths [Å]: Th(1)–Cl(1) 2.68070(8) , Th(1)–Cp<sub>cent</sub> 2.5440(19).



**Figure S23.** Solid-state molecular structure of **2-U** measured at 150 K. Ellipsoids set at 50 % probability; hydrogen atoms and lattice solvent removed for clarity. C, Si and U atoms are shown as grey, orange, and green respectively.

	[Th(Cp') <sub>3</sub> {Si(SiMe <sub>3</sub> ) <sub>3</sub> }] (2-Th)	[U(Cp') <sub>3</sub> {Si(SiMe <sub>3</sub> ) <sub>3</sub> }] (2-U)
An(1)-Si(1)	3.1191(8) Å	3.0688(8) Å
Mean $An(1)$ – $Cp_{cent}$	2.5392(24) Å	2.4715(26) Å
Mean An(1)–Si(1)–Si	116.48(6)°	116.97(7)°
Mean $Cp_{cent}$ -An(1)-Si(1)	96.93(5)°	96.66(7)°

 Table S2. Selected bond distances and angles for complexes 2-Th and 2-U.

### **10. Quantum chemical calculations**

The Gaussian 16 software package,<sup>13</sup> revision C.01, was used for all density functional theory, excluding the NMR calculations (see below). The hybrid density functional approximation, PBE0,<sup>14,15</sup> was employed with Grimme's D3 dispersion corrections and the Becke-Johnson damping parameters (D3-BJ).<sup>16–20</sup> Dunning's correlation consistent basis sets of polarised triple-ζ quality were used for H, C, and Si atoms.<sup>21–24</sup> Stuttgart-Bonn small-core (60 electrons) relativistic pseudopotentials and associate segmented basis sets were used for the actinide atoms.<sup>25–27</sup> Initial geometries were taken from the single crystal XRD structures and optimised with no symmetry constraints. The quadratically convergent SCF procedure (SCF=XQC) was used in the case of **2-U** to assist with the electronic convergence. Otherwise, default settings were used for the optimisations and analysis of the harmonic vibrational frequencies confirmed that energetic minima were located. Subsequently, single point energy calculations were done with the all-electron SARC basis sets<sup>28–30</sup> for the actinide atoms and the second-order Douglas-Kroll-Hess (DKH2) Hamiltonian to account for scalar relativistic effects.<sup>31–33</sup> Bonding analyses were performed on the all-electron electronic structures.

The Natural Bond Orbitals (NBO 7.0) software package, integrated with Gaussian 16, was used to compute natural localised molecular orbitals (NLMOs) to analyse the actinidesilicon bonding orbitals.<sup>34,35</sup> WFX files generated from Gaussian 16 were used for the quantum chemical topology (QCT) analysis, including QTAIM and IQA analysis, which was performed with the AIMAII software package.<sup>36</sup> The IQA analysis was implemented using encomp=4 and WFX file were edited to include the appropriate <Model> tag.

The NMR chemical shifts were computed with the Amsterdam Density Functional Theory (ADF) programme.<sup>37,38</sup> Spin-orbit coupled, single-point calculations, using the optimised geometries described above, employed the PBE0 hybrid functional. All-electron Slater-type orbital triple- $\zeta$  quality basis sets (TZ2P) were employed for the An and Si atoms, and double- $\zeta$  quality basis sets (DZP) were employed for C and H atoms, in conjunction with the two-component zero-order regular approximation (ZORA) Hamiltonian.<sup>39–43</sup> The silicon chemical shifts are reported relative to tetramethylsilane (TMS).

Complex	$\nabla^2 \rho_{BCP}$	$G_{ m BCP}$	$V_{\rm BCP}$	$-(G_{\rm BCP}/V_{\rm BCP})$	[ <i>ε</i> (r)]
1-Th	-0.001	0.013	-0.025	0.497	0.0001
<b>1-</b> U	0.001	0.014	-0.027	0.504	0.0005

Table S3. Additional QTAIM metrics for the An-Si bond critical point for 2-An.

**Table S4.** Optimized Cartesian coordinates (Å) and corresponding SCF energies for **2-An** at the PBE0/ECP60MWB/cc-pVTZ level of theory.

		2-Th				<b>2-</b> U	
Energy: -3729.8418020 Hartrees				Energ	gy: -3798.680	1738 Hartree	es
Th	-0.439059	0.000118 0.001	143	U	-0.426250	0.000124	0.000952
Si	2.632164	-0.000748 -0.000	816	Si	2.585450	-0.000238	-0.000570
Si	3.684851	-1.683637 -1.303	813	Si	3.663646	1.996768	-0.736294
Si	3.684661	1.969802 -0.804	757	Si	3.664493	-0.360640	2.096425
Si	3.684583	-0.289813 2.109	001	Si	3.664832	-1.637392	-1.359251
Si	-2.993606	-2.052715 -2.790	621	Si	-2.985731	3.418122	-0.276261
Si	-2.987932	3.447011 -0.383	084	Si	-2.992285	-1.470337	3.090899
Si	-2.997044	-1.390918 3.169	349	Si	-2.987571	-1.947626	-2.818195
С	3.666226	-1.278036 -3.155	147	С	3.650913	3.360435	0.594823
Н	2.667015	-1.381779 -3.587	954	Н	2.646001	3.782854	0.748220
Н	4.327438	-1.978405 -3.679	412	Н	4.311005	4.183565	0.272789
Н	4.022557	-0.264941 -3.364	272	Н	4.019026	2.998218	1.567294
C	2.869188	-3.386294 -1.155	018	С	2.865935	2.791897	-2.272216
H	2.939102	-3.795294 -0.142	488	Н	2.931913	2.143710	-3.160094
H	3.379295	-4.084433 -1.829	592	Н	3.397884	3.729479	-2.506638
Н	1.812881	-3.360356 -1.435	133	Н	1.805754	3.038535	-2.112122
C	5.497702	-1.965886 -0.844	484	С	5.486366	1.752493	-1.218037
H	6.095036	-1.058045 -0.957	707	Н	6.085991	1.361965	-0.383627
Н	5.917758	-2.734892 -1.504	496	Н	5.912462	2.724053	-1.521695
Н	5.604147	-2.315832 0.186	447	Н	5.590747	1.059633	-2.066860
C	2.868160	2.692307 -2.352	902	C	2.866889	0.569846	3.554234
H	2.942431	2.021633 -3.214	398	Н	2.927591	1.663103	3.436053
H	3.374669	3.628197 -2.617	822	Н	3.402269	0.306971	4.482265
H	1.810530	2.916729 -2.191	210	Н	1.808402	0.302329	3.690325
C	5.497993	1.714345 -1.278	436	С	5.487386	0.179086	2.125726
H	6.096374	1.361324 -0.434	918	Н	6.086791	-0.347795	1.369744
H	5.917205	2.669874 -1.617	021	Н	5.913320	-0.044856	3.118767
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Н	0.274270 -1.304086	3.109909	Н	0.302266	-1.937145	-2.681271

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