Electronic Supplementary Information

Inhibition of C(2)-H/D Exchange of a Bis(imidazolium) Dication Upon Complexation with Cucubit[7]uril

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Materials

Cucurbit[7]uril was synthesized by the reported method of Day *et al.*¹ The acetate and phosphate buffer solutions (total buffer concentration of 0.05 M for each kinetic experiment) were prepared by the requisite addition of DCl (Aldrich, 35 wt.% in D₂O) to D₂O solutions of sodium acetate and sodium phosphate (Aldrich), respectively. The ionic strength was adjusted to 0.2 M using NaCl.

Synthesis of [BMIX]Br₂:

α,α'-Bis(3-(1-methylimidazolium))-*p*-xylene was synthesized by using a modified literature method.² 1-methylimidazole (Aldrich, 1.0 g, 12 mmol) was heated with α,α'-dibromo-*p*-xylene (Aldrich, 1.58 g, 6.0 mmol) in THF under reflux for 36 hours to give an off-white precipitate. The crude product was filtered, washed with THF and ether, and dried in a vacuum oven to give a white power (2.4 g, 93% yield). M.p. 234-236 °C (dec.). ¹H NMR (D₂O, 400 MHz) δ 8.68 (s, 2H), 7.38 (br s, 8H), 5.34 (s, 4H), 3.80 (s, 6H) ppm. (Lit.³ for [BMIX]I₂ ⁻¹H NMR (DMSO-d₆) δ 9.20 (s, 2H, H₂), 7.75 (s, 2H, H₄), 7.70 (s, 2H, H₅), 7.45 (s, 4H, H_{Ar}), 5.41 (s, 4H, H_α), 3.84 (s, 6H, CH₃) ppm). ¹³C NMR (D₂O, 100 MHz) δ 136.17, 134.60, 129.27, 123.87, 122.29, 52.30, 35.76 ppm. (Lit.³ for [BMIX]I₂ ⁻¹C NMR (D₂O, 100 MHz) δ 138.0, 134.8, 129.6, 124.1, 122.5, 52.6, 36.1 ppm). **ESI-MS:** m/z = 347.1 and 349.1 [M-Br]⁺ (calc. 347.1 and 349.1), m/z = 267.2 [M-2Br]²⁺ (calc. 267.2), shown in Fig. S1.



Fig. S1 Electrospray ionization mass spectrum of [BMIX]Br₂.



Fig. S2 Electrospray ionization mass spectrum of the {BMIX•CB[7]}²⁺ guest-host complex. Single-charged peak observed at m/z = 1509 (calculated 1509) for {(BMIX+Br)•CB[7]}⁺ (isotopic pattern shown enlarged in insert). Double-charged peak observed at m/z 715 (calculated 715) for {BMIX•CB[7]}²⁺.

Determination of the Guest-Host Stability Constant:

The stoichiometry of the guest-host complex formed between BMIX²⁺ and CB[7] was determined to be 1:1 based on a Job's plot (Fig. S3). The absorbance at 220 nm was monitored as the concentrations of CB[7] and BMIX²⁺ were varied, keeping [CB[7]] + $[BMIX^{2+}] = 1.0 \text{ mM}$. The maximum is located at $[CB[7]]/([BMIX^{2+}] + [CB[7]]) = 0.50$, indicating a 1:1 stoichiometry.



Fig. S3 Job's plot based on UV-visible continuous variation titration with $[CB[7]] + [BMIX^{2+}] = 1.0 \text{ mM}$ in aqueous solution, indicating a 1:1 complex formation between CB[7] and $BMIX^{2+}$.

The guest-host stability constant was estimated to be in the order of $10^8 - 10^{10}$ M⁻¹, as a similar guest, the *p*-xylenediammonium dication was reported to have a binding constant with CB[7] of 1.84 x 10^9 M⁻¹. The (trimethylammonio)methylferrocene (FcTMA⁺) cation

(as the iodide salt), with a binding constant with CB[7] of $(3.31 \pm 0.62) \times 10^{11}$ M^{-1,4} was successfully employed as the competitor. The ¹H NMR spectrum of a D₂O (0.1 M NaCl) solution of 1.8 mM FcTMA⁺ and 22.5 mM BMIX²⁺, with a limiting quantity of CB[7] (about 2.1 mM) was recorded at 25 °C. The concentrations of the free and bound BMIX²⁺ and FcTMA⁺ were determined from integrations of their respective proton resonances (**Fig. S4**).

 $[FcTMA^+]_{total} = 1.82 \text{ mM}$ (integration for both bound and free trimethyl group protons is 9), $[CB[7]]_{total} = 1.82 \times 15.60/14 = 2.03 \text{ mM}$ (integration for 14 methylene protons of CB[7] is 15.60);

 $[BMIX^{2+}]_{bound} = 1.82 \times 1.58/4 = 0.72 \text{ mM}$ (Integration for bound-guest 4 aromatic proton is 1.58);

 $[BMIX^{2+}]_{free} = 1.82 \times (97.46 - 1.58)/8 = 21.81 \text{ mM}$ (Integration for free-guest's four aromatic protons and the free and bound guest's four ethylene protons is 97.46, and with the integration of the four protons of the bound ethylene equaling 1.58);

Therefore, $[CB[7]-BMIX^{2+}]_{complex} = [BMIX^{2+}]_{bound} = 0.72 \text{ mM};$ $[CB[7]-FcTMA^+]_{complex} = [CB[7]]_{total} - [CB[7]-BMIX^{2+}]_{complex} = 2.03 - 0.72 = 1.31 \text{ mM};$ and $[FcTMA^+]_{free} = [FcTMA^+]_{total} - [CB[7]-FcTMA^+]_{complex} = 1.82 - 1.31 = 0.51 \text{ mM}.$

 $K_{\rm BMIX}/K_{\rm FcTMA} = [CB[7]-BMIX^{2+}]_{\rm complex} \times [FcTMA^{+}]_{\rm free}/([CB[7]-FcTMA^{+}]_{\rm complex} \times [BMIX^{2+}]_{\rm free})$ = 0.72×0.51/(1.31×21.81) = 0.0128 and $K_{\rm CB[7]-FcMA} = (3.31 \pm 0.62) \times 10^{11} \text{ M}^{-1}$ Therefore, $K_{\rm BMIX} = (4.3 \pm 0.8) \times 10^{9} \text{ M}^{-1}$



Fig. S4 ¹H NMR spectrum of the competition between $BMIX^{2+}$ (22.5 mM) and $FcTMA^{+}$ (1.8 mM) for CB[7] (2.1 mM,) in D₂O.

Kinetics of H/D exchange monitored by ¹H NMR spectroscopy:

Representative ¹H NMR spectra of BMIX²⁺ in the absence and in the presence of CB[7] obtained during the hydrogen/deuterium exchange for the C(2)-proton at different p*D* conditions (buffered by DOAc/OAc⁻ or DPO₄/D₂PO₄⁻, or PO₄³⁻/DPO₄²⁻ in D₂O, I = 0.20 (NaCl)) are given below. The xylyl methylene protons' resonance in BMIX²⁺ is used as an internal reference resonance for obtaining the integration of the C(2)-protons. All of

the ¹H NMR spectra were recorded on an Avance 400MHz NMR spectrometer and, in order to acquire accurate integrals for the C(2)-proton resonance, a relaxation delay between pulses of $d_1 = 75$ s (> 5T₁) was used.



Fig. S5 Representative ¹H NMR spectra at 400 MHz of BMIX²⁺ in the absence CB[7] obtained during deuterium exchange of C(2)-proton (in D₂O, pD = 5.2 buffered by DOAc/OAc⁻, I = 0.2 (NaCl)). From top down, H/D exchange proceeded for 0, 4, 18, and 34 days.



Fig. S6 Representative ¹H NMR spectra at 400 MHz of BMIX²⁺ in the presence of 1.1 equiv. CB[7] obtained during deuterium exchange of C(2)-proton (in D₂O, pD = 9.5 buffered by DPO₄²⁻/D₂PO₄⁻, I = 0.2 (NaCl)). From top down, H/D exchange proceeded for 20 min, 7.5 hours, 2 days, and 3 days.

First-order rate constants determination by semilogarithmic plots:

Values of the reaction progress, *R*, were calculated from the integration of the resonances of C(2)-protons, compared with the internal reference of the methylene protons (H(α)), at zero time and time *t*, according to the equations below:

 $R = (I_{2H})_t/((I_{2H})_0) = (I_{2H})_t/2$, as the reference methylene proton (H(α)) resonance integrated to four protons, and the initial integration for the C(2)-protons is two, relative to the four methylene (H(α)) protons;

 $\ln R = -k_{\rm ex}t;$

Therefore, the first-rate constants can be determined from the slopes of the linear semilogarithmic plots of reaction progress against reaction time (Fig. S7 and S8).



Fig. S7 Plots of ln*R* against time for the C(2)-H/D exchange reactions of BMIX²⁺ at pD = 5.16 (\Box) and 6.17 (Δ) and {BMIX•CB[7]}²⁺ at pD = 8.81 (\blacktriangle) and 9.51 (\blacksquare).



Fig. S8 Plots of ln*R* against time for the C(2)-H/D exchange reactions of BMIX²⁺ at p*D* = 7.44 (\circ) and 8.07 (∇) and {BMIX•CB[7]}²⁺ at p*D* = 10.15 (\bullet).

Table S1. First-order rate constants, k_{ex} , for deuterium exchange of the C(2)-protons of BMIX²⁺ in the absence and in the presence of 1.1 equiv of CB[7] in D₂O at 25 °C and I = 0.2 (NaCl) in various pD buffer solutions.

Species	10 ³ [Substrate] (M)	Buffer	pD	$k_{\mathrm{ex}}(\mathrm{s}^{-1})$
	2.0	$OAc^{-}/DOAc$ $f_{\rm B} = 0.5$	5.16	2.98×10^{-7}
DMIV ²⁺	2.0	$OAc^{-}/DOAc$ $f_{\rm B} = 0.9$	6.17	2.47 × 10 ⁻⁶
DIVITA	2.0	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.2$	7.44	6.43 × 10 ⁻⁵
	2.0	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.8$	8.07	2.26×10^{-4}
{BMIX•CB[7]} ²⁺	0.5	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.9$	8.35	1.23 x 10 ⁻⁴
	1.0	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.9$	8.44	1.15 x 10 ⁻⁵
	5.0	$DPO_4^{2-}/D_2PO_4^{-}$ $f_B = 0.9$	8.74	1.21 x 10 ⁻⁶
	2.0	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.9$	8.81	8.64 × 10 ⁻⁷
	2.0	$DPO_4^{2^-}/D_2PO_4^{-1}$ $f_B = 0.95$	9.51	5.11 × 10 ⁻⁶
	2.0	PO_4^{3-}/DPO_4^{2-} $f_B = 0.1$	10.50	4.54×10^{-5}

Note: Total buffer concentration is 0.05 M in D_2O . f_B is the fraction of the base form of the buffer.

Determinations of the second-order rate constants:

The second-order rate constant, k_{OD} , is calculated from the *y*-axis intercept of the linear fits with a fixed slope of unity (**Fig. 3**) by using the first-order rate constants and p*D* conditions according to the equation below,⁵

 $\log k_{\rm ex} = \log (k_{\rm DO} K_{\rm W} / \gamma_{\rm OL}) + pD$

where $K_W = 14.87$, and under our experimental conditions, the activity correction for deuterium oxide is $\gamma_{OL} = 0.83$.⁵

Ab Initio Energy-Minimized Calculations of the Structure of {BMIX•CB[7]}²⁺

The structure of the {BMIX•CB[7]}²⁺ guest-host complex was computed by energy minimizations using Gaussian 03, Revision C.02 programs⁶ run on the computing facilities of the High Performance Virtual Computing Laboratory (HPVCL) at Queen's University. The structure of the complex was originally constructed using ChemDraw and Chem 3D (ChemOffice 7.0, CambridgeSoft) programs and imported into Gaussian 03. The basis set used for the calculations was HF/3-21G**. The structure was minimized to final energy of -4995.49632663 A.U. A picture of the guest-host complex, with the Cartesian axes added, is given in Figure S9. The Cartesian coordinates of the atoms are given in Table S2.



Fig. S9 A "ball and bond" picture of the energy-minimized structure of {BMIX •CB[7]}²⁺ showing the Cartesian axes (z is vertical and y points to the right).

Center Number	Atomic Number	Atomic Type	Coord X	dinates (Ang: Y	stroms) Z
1	6	0	-4.164528	-4.020472	0.733153
2	6	0	-2.916710	-4.988775	0.674664
3	7	0	-2.070802	-4.484570	1.730725
4	6	0	-2.572476	-3.357731	2.333589
5	7	0	-3.814555	-3.120560	1.806112
б	7	0	-4.189048	-3.445101	-0.595117
7	6	0	-3.182779	-3.909140	-1.403407
8	7	0	-2.425433	-4.794791	-0.672500
9	8	0	-2.052205	-2.739964	3.241083
10	8	0	-3.044172	-3.660304	-2.583830
11	6	0	0.614558	-5.779890	0.322976
12	6	0	2.138582	-5.422393	0.096854
13	7	0	2.456807	-4.607937	1.246321
14	6	0	1.369631	-4.367346	2.052146
15	7	0	0.303680	-5.060411	1.534800
16	7	0	-0.018658	-5.289200	-0.886053
17	6	0	0.856247	-4.654188	-1.726719
18	7	0	2.108504	-4.730175	-1.174062
19	8	0	1.371566	-3.728551	3.082465
20	8	0	0.595567	-4.181557	-2.818054
21	6	0	-0.930945	-5.188404	2.280699
22	6	0	-1.384137	-5.592568	-1.28913
23	6	0	4.914930	-3.105181	-0.371371
24	6	0	5.553445	-1.667676	-0.522426
25	1	0	5.26/4/2	-1.0545/4	0./55838
26	6	0	4.562591	-1.8/2556	1.606201
27	7	0	4.350829	-3.066104	0.958/94
28		0	3.958660	-3.14293/	-1.456225
29	6	0	3.8/8812	-1.961388	-2.14/181
30	/	0	4.842400	-1.120608	-1.050952
31 22	8	0	4.203984	-1.022/23	2./55290
3⊿ 22	0	0	5.12/004	-1.757694	-3.0010/5
22	0 C	0	4 902056	1.904940	-0.033901
25	0 7	0	4.003950	2.202093 2.245140	
35	6	0	4.125262	2 102160	1 300000
30 27	0	0	4.330001 E 106110	1 101201	1.399005
30	7	0	J.190110 A 949221	1 226200	-1 760829
30	6	0	2 0/00/0	2 156522	-2 280111
40	6	0	-0.268100	0 730846	1 218059
40	6	0	0 446963	-0 360945	0 738088
42	6	0	0.781709	-0 443063	-0 603528
43	6	0	0.411536	0.443003	-1 485248
44	6	0	-0 305822	1 640579	-1 007521
45	6	0	-0 639843	1.726322	0 332592
46	6	0	-0 670964	0 858308	2 682925
47	5 7	0	0.395838	0.332544	3.559388
48	, 6	0	0.725986	0.486802	-2,966917
49	5 7	0	-0.274307	-0.395183	-3.618387
50	, 6	0	1.509444	0.979725	3.875794
51	5 7	0 0	2.267922	0.171206	4.595778

Table S2.	Coordinates of the atom	ms in energ	y-minimized str	ucture of {BM	$IX \cdot CB[7]$ ²⁺ .

Center	Atomic	Atomic	Coord	dinates (Ang	stroms)
Number	Number	Туре	Х	Y	Z
52		 0	1 622021		4 725804
53	6	0	0 447040	-0 957412	4 086890
54	6	0	-1 638772	-0 130066	-3 737432
55	6	0	-2 187467	-1 215929	-4 303461
56	7	0	-1 156217	-2 124470	-4 536239
57	, 6	0	-0 023434	-1 603872	-4 092968
58	6	0	3 619625	0 460319	5 120797
59	6	0	-1 324737	-3 462904	-5 139041
60	1	0	-0 448305	-4 043858	-4 916282
61	1	0	-1 460856	-3 361601	-6 204693
62	1	0	-2 181997	-3 917747	-4 677956
63	1	0	3 595466	0 419956	6 198501
64	1	0	3 916772	1 433314	4 777643
65	1	0	4 285658	-0 281019	4 716085
66	1	0	-3 201164	-1 442451	-4 507419
67	1	0	2 074207	-1 880911	5 216892
68	1	0	0 925535	-2 081094	-4 061347
69	1	0	-2 077502	0 779310	-3 405028
70	- 1	0	-0.332256	-1.661439	3,919946
71	- 1	0	1.745160	1,968698	3,561976
72	- 1	0	1 693726	0 064923	-3 156665
73	1	0	0.676546	1,461920	-3.418423
74	- 1	0	-0.611031	2.394612	-1.695266
75	1	0	1.324610	-1.290705	-0.966343
76	1	0	-1.569008	0.304340	2.900663
77	1	0	-0.846668	1.888303	2.938515
78	1	0	-1.174322	2.581281	0.678896
79	1	0	0.750306	-1.137644	1.409012
80	7	0	3.951325	3.367023	-1.745360
81	8	0	3.948307	1.957027	2.523710
82	8	0	3.314867	1.879882	-3.389419
83	6	0	5.812354	0.211373	1.210331
84	б	0	5.242453	0.083470	-2.367914
85	б	0	3.792339	-4.211297	1.653914
86	б	0	3.285663	-4.340221	-1.922372
87	б	0	1.890440	5.578378	-0.381028
88	6	0	0.339525	5.868636	-0.282169
89	7	0	-0.025318	5.245335	0.972164
90	6	0	1.010019	4.553355	1.553085
91	7	0	2.139705	4.794058	0.810797
92	7	0	2.004440	4.863130	-1.630183
93	6	0	0.792523	4.604748	-2.218151
94	7	0	-0.178421	5.223421	-1.467701
95	8	0	0.957807	3.916809	2.589317
96	8	0	0.609329	3.998118	-3.252780
97	6	0	-3.176362	5.042248	-0.026659
98	6	0	-4.420842	4.070773	0.096332
99	7	0	-4.232358	3.477058	1.398430
100	6	0	-3.053701	3.837017	1.996618
101	7	0	-2.430299	4.752902	1.182027
102	7	0	-2.552060	4.608302	-1.253614
103	6	0	-3.139003	3.488106	-1.791860
104	7	0	-4.240641	3.180529	-1.036276

NumberNumberTypeXYZ10580 -2.650942 3.466615 3.079270 10680 -2.779395 2.919634 -2.844405 10760 -1.573461 5.352427 -1.972657 10960 3.460905 4.477456 1.313963 11060 3.247415 4.513684 -2.289697 11160 -5.238922 2.241543 -1.527433 11260 -5.27965 -2.625600 -1.127647 11360 -5.267965 -2.605452 $.2446167$ 11560 -5.989667 -0.818751 0.599350 11660 -5.934631 0.752846 0.439010 11770 -5.198292 1.230818 1.549311 11870 -4.964986 -0.202805 -1.489907 12170 -5.9477063 0.224635 2.279305 12380 -4.528944 0.292397 -0.618726 12440 0.784866 0.3278811 3.250113 12510 -5.947706 -0.284739 0.045925 12610 -1.51262966 -6.284739 0.045925 12710 0.429189 -6.835872 0.448570 12810 -7.67633 2.217440 0.845270 12910 -1.51262966	Center Atomic Atomic			Coordinates (Angstroms)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Number	Number	Туре	Х	Ŷ	Z
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	105	8	0	-2.650942	3.466615	3.079270
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	106	8	0	-2.779395	2.919634	-2.804405
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	107	6	0	-1.277569	5.491724	1.666037
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	108	6	0	-1.533461	5.352427	-1.972657
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	109	6	0	3.460905	4.477456	1.313963
11160 -5.238982 2.241543 -1.527433 11260 -5.173850 2.59872 2.064011 11360 -5.267965 -2.625600 -1.127647 11460 -4.740100 -2.207545 2.446167 11560 -5.85967 -0.818751 0.599350 11660 -5.85967 -0.818751 0.599350 11660 -5.934431 0.752846 0.439010 11770 -5.138222 1.230818 1.584311 11970 -5.313863 -1.249934 -0.669046 12060 -4.964936 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.29237 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.02544739 0.442874 12810 -1.183223 -6.237166 2.388663 13010 -1.446284 -5.417252 -2.348721 13310 5.670284 -2.948737 -0.623161 13510 6.615427 -1.601494 -0.786204 13610	110	6	0	3.247415	4.513684	-2.289697
11260 -5.173850 2.598872 2.064011 11360 -5.267965 -2.625600 -1.127647 11460 -4.740100 -2.207545 2.446167 11560 -5.859067 -0.818751 0.599380 11660 -5.93420 1.230818 1.584311 11770 -5.198292 1.230818 1.584311 11870 -4.986933 -0.969476 1.741871 11970 -5.313863 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489974 12170 -5.301135 0.964217 -0.846999 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -1.162926 -6.284739 0.045925 12810 -1.163223 -6.237816 2.388663 13010 -1.446828 -5.417252 -2.348721 13310 5.627088 -3.910189 -0.463937 13310 6.6376251 -1.074537 13310 6.637844 0.238275 0.975855 13810 6.677634	111	6	0	-5.238982	2.241543	-1.527433
11360 -5.267965 -2.625600 -1.127647 11460 -4.740100 -2.207545 2.446167 11560 -5.934431 0.752846 0.439010 11660 -5.934431 0.752846 0.439010 11770 -5.138292 1.230818 1.584311 11870 -4.966933 -0.969476 1.741871 11970 -5.313863 -1.249934 -0.666946 12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.866999 12260 -4.570763 0.224635 2.779305 12380 -3.861894 0.357861 3.250113 12510 -5.094706 -4.524034 0.946520 1261 0.318226 -6.025444 0.845570 12710 0.429189 -6.835872 0.442874 12810 -1.183223 -6.237816 2.358663 13010 -1.446828 -5.417252 -2.348721 13210 -6.636251 -1.074537 13310 6.570763 2.011804 -0.716234 13510 6.570763 2.011804 -0.786204 13610 5.670254 0.242336 2.276266 13910 4.776088 0.524444 <td>112</td> <td>6</td> <td>0</td> <td>-5.173850</td> <td>2.598872</td> <td>2.064011</td>	112	6	0	-5.173850	2.598872	2.064011
1146 -4.740100 -2.207545 2.446167 11560 -5.893607 -0.818751 0.599350 11770 -5.198292 1.230818 1.584311 11870 -4.986933 -0.969476 1.741871 11970 -5.313863 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489907 12170 -5.30135 0.964217 -0.646099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.845570 12710 0.42919 -6.835872 0.442874 12810 -7.784857 -6.284739 0.045925 12910 -1.183223 -6.237816 2.358663 13110 -6.6570763 2.011804 -0.786204 13310 6.615427 -1.681184 -0.711621 13510 6.670254 0.242336 2.276266 13910 4.97608 0.22375 0.975855 13810 2.965119 -4.155047 -2.338163 14410 3.995715	113	6	0	-5.267965	-2.625600	-1.127647
11560 -5.859067 -0.818751 0.599350 11660 -5.934431 0.752846 0.439010 11770 -5.198292 1.230818 1.584311 11870 -4.996933 -0.969476 1.741871 11970 -5.313163 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.845570 12710 0.429189 -6.835872 0.442874 12810 -7.743807 -6.237816 2.388663 13010 -1.183223 -6.237816 2.388633 13010 -1.571688 -6.636251 -1.074537 13310 5.670763 2.011804 -0.786204 13510 6.570763 2.011804 -0.786204 13610 5.670254 0.242236 2.276266 13710 6.657075 -2.937815 -2.372626 13810 5.670254 0.242237 -2.372626 13810 2	114	6	0	-4.740100	-2.207545	2.446167
11660 -5.934431 0.752464 0.439010 11770 -5.192292 1.230818 1.584311 11970 -5.313663 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.8660946 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.845570 12710 0.429189 -6.284739 0.045925 12910 -1.183223 -6.237816 2.358663 13010 -1.743804 -4.778337 3.258486 13110 -1.446828 -5.417252 -2.348721 13210 5.670288 -3.910189 -0.6623161 13310 5.670284 -3.910189 -0.6231763 13410 6.615427 -1.681184 -0.711621 13510 6.70763 2.011804 -0.778624 13610 5.472526 -2.471920 13710 6.867844 0.238275 -2.928626 13810 2.965119 <td< td=""><td>115</td><td>6</td><td>0</td><td>-5.859067</td><td>-0.818751</td><td>0.599350</td></td<>	115	6	0	-5.859067	-0.818751	0.599350
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	116	6	0	-5.934431	0.752846	0.439010
11870 $-4,986933$ -0.96976 1.741871 11970 -5.313863 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.84557 12710 0.429189 -6.835872 0.442874 12810 -1.83223 -6.237816 2.358663 13010 -0.743804 -4.778337 3.258486 13110 -1.571688 -6.632551 -1.074537 13310 5.627088 -3.910189 -0.463937 13410 6.577063 2.011804 -0.775855 13810 5.67068 0.2242336 2.76266 13910 4.776088 0.2242375 2.975265 13810 5.67763 2.011804 -3.38158 14010 6.319567 0.667377 -2.932689 14110 3.73296 -3.938813 2.694099 14210 4.727678	117	7	0	-5.198292	1.230818	1.584311
11970 -5.313863 -1.249934 -0.669046 12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224355 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.284739 0.442874 12810 2.784857 -6.284739 0.045925 12910 -1.183223 -6.237816 2.358663 13010 -1.571688 -6.636251 -1.074537 13310 5.627088 -3.910189 -0.463937 13410 6.515427 -1.681184 -0.711621 13510 6.570763 2.011804 -0.786204 13610 5.670254 0.242336 2.276266 13910 4.776088 0.5282767 -2.932689 14410 3.79426 -3.938813 2.694099 14210 4.955119 -4.155047 -2.932689 14410 3.995715 -5.155041 -1.902432 14510 -2.972807 -5.97486 14610 -3.732807	118	7	0	-4.986933	-0.969476	1.741871
12060 -4.964986 -0.202805 -1.489907 12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.845570 12710 0.429189 -6.284739 0.045925 12910 -1.183223 -6.237816 2.358663 13010 -0.743804 -4.778337 3.258486 13110 -1.446828 -5.417252 -2.348721 13310 5.627088 -3.910189 -0.463937 13310 5.670254 0.2423762 0.975855 13810 6.570763 2.011804 -0.786204 13710 6.867884 0.238275 0.975855 13810 4.776088 0.52444 -3.38158 14010 3.995715 -5.156041 -1.902432 14110 3.995715 -5.156041 -1.902432 14410 3.995715 -5.156041 -1.902432 14510 -0.724877 -2.932689 14410 -3.978677 -2	119	7	0	-5.313863	-1.249934	-0.669046
12170 -5.301135 0.964217 -0.846099 12260 -4.577063 0.224635 2.279305 12380 -4.528994 -0.292397 -2.618726 12480 -3.861894 0.357881 3.250113 12510 -5.094706 -4.524034 0.946520 12610 -3.162926 -6.025444 0.845570 12710 0.429189 -6.835872 0.442874 12810 2.784857 -6.237816 2.358663 13010 -1.183223 -6.237816 2.358663 13110 -1.743804 -4.778337 3.258486 13310 5.67088 -3.910189 -0.463937 13310 5.670254 2.928275 0.975858 13410 6.615427 -1.681184 -0.711621 13510 5.670254 0.242336 2.276266 13910 4.776088 0.52444 -3.338158 14010 3.995715 -5.156041 -1.902432 14110 3.995715 -5.156041 -1.902432 14410 2.997312 4.24284 2.59336 15110 -1.183746 5.196457 2.692655 15110 -1.810774 6.918541 -0.271712 14410 3.995715 </td <td>120</td> <td>6</td> <td>0</td> <td>-4.964986</td> <td>-0.202805</td> <td>-1.489907</td>	120	6	0	-4.964986	-0.202805	-1.489907
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	121	7	0	-5.301135	0.964217	-0.846099
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	122	6	0	-4.577063	0.224635	2.279305
12480 -3.861894 0.357881 3.250113 125 10 -5.094706 -4.524034 0.946520 126 10 -3.162926 -6.025444 0.845570 127 100.429189 -6.835872 0.442874 128 10 -1.183223 -6.237816 2.358663 130 10 -0.743804 -4.778337 3.258486 131 10 -1.446828 -5.417252 -2.348721 132 10 -1.571688 -6.636251 -1.074537 133 10 5.627088 -3.910189 -0.4639371 134 10 6.615427 -1.681184 -0.711621 135 10 6.570763 2.011804 -0.786204 136 10 5.670254 0.242336 2.276266 139 10 4.776088 0.052444 -3.338158 140 10 3.734296 -3.938813 2.694099 142 10 4.95620 -5.055787 1.523026 143 10 2.965119 -4.155047 -2.932689 144 10 3.995715 -5.156041 -1.902432 144 10 3.995715 -5.156041 -1.902432 144 10 -1.490460 6.550972 1.607243 150 10 -1.810174 6.918541 -0.271712 147 <td>123</td> <td>8</td> <td>0</td> <td>-4.528994</td> <td>-0.292397</td> <td>-2.618726</td>	123	8	0	-4.528994	-0.292397	-2.618726
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	124	8	0	-3.861894	0.357881	3.250113
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	125	1	0	-5.094706	-4.524034	0.946520
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	126	1	0	-3.162926	-6.025444	0.845570
128102.784857 -6.284739 0.04592512910 -1.183223 -6.237816 2.35866313010 -0.743804 -4.778337 3.258486 13110 -1.446828 -5.417252 -2.348721 13210 -1.571688 -6.636251 -1.074537 13310 5.627088 -3.910189 -0.463937 13410 6.615427 -1.681184 -0.711621 13510 6.570763 2.011804 -0.786204 13610 5.494525 4.210630 -0.623161 13710 6.867884 0.238275 0.975585 13810 5.670254 0.242336 2.276266 13910 4.776088 0.052444 -3.338158 14010 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 0.092187 6.918541 -0.271712 14610 -5.372807 4.574058 0.036973 14910 -1.490460 6.550972 1.607243 15010 -1.518458 4.973960 -2.981107 15210 -1.518458 <td>127</td> <td>1</td> <td>0</td> <td>0.429189</td> <td>-6.835872</td> <td>0.442874</td>	127	1	0	0.429189	-6.835872	0.442874
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	128	1	0	2.784857	-6.284739	0.045925
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	129	1	0	-1.183223	-6.237816	2.358663
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	130	1	0	-0.743804	-4.778337	3.258486
13210 -1.571688 -6.636251 -1.074537 133 10 5.627088 -3.910189 -0.463937 134 10 6.615427 -1.681184 -0.711621 135 10 6.570763 2.011804 -0.786204 136 10 5.494525 4.210630 -0.623161 137 10 6.867884 0.238275 0.975585 138 10 5.670254 0.242336 2.276266 139 10 4.776088 0.052444 -3.338158 140 10 6.319567 0.067356 -2.471920 141 10 3.734296 -3.938813 2.694099 142 10 4.455620 -5.055787 1.523026 143 10 2.965119 -4.155047 -2.932689 144 10 3.995715 -5.156041 -1.902432 145 10 2.501869 6.466887 -0.387275 146 10 0.092187 6.918541 -0.271712 147 10 -3.443141 6.086282 -0.077071 148 10 -1.139746 5.196457 2.692685 151 10 -1.810174 6.398177 -1.966035 153 10 4.087479 5.351104 1.190975 154 10 3.357942 4.244284 2.359336 155	131	1	0	-1.446828	-5.417252	-2.348721
13310 $5.62/088$ -3.910189 $-0.48393/$ 13410 6.615427 -1.681184 -0.711621 13510 6.570763 2.011804 -0.786204 13610 5.494525 4.210630 -0.623161 13710 6.867884 0.238275 0.975585 13810 5.670254 0.242336 2.276266 13910 4.776088 0.052444 -3.338158 14010 6.319567 0.067356 -2.471920 14110 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 -5.372807 4.574058 0.036973 14910 -1.139746 5.196457 2.692685 15110 -1.518458 4.973960 -2.981107 15210 -1.810174 6.398177 -1.966035 15310 2.997312 4.244284 2.359336 15510 2.997312 4.269093 -3.308429 15610 3.908641 5.368534 -2.258782 15710 -4.994455 <td>132</td> <td>1</td> <td>0</td> <td>-1.571688</td> <td>-6.636251</td> <td>-1.074537</td>	132	1	0	-1.571688	-6.636251	-1.074537
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	133	1	0	5.62/088	-3.910189	-0.46393/
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	134	1	0	6.615427	-1.681184	-0./11621
13610 5.494525 4.210630 -0.623161 13710 6.867884 0.238275 0.975585 13810 5.670254 0.242336 2.276266 13910 4.776088 0.052444 -3.338158 14010 6.319567 0.067356 -2.471920 14110 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 0.092187 6.918541 -0.271712 14710 -3.443141 6.086282 -0.077071 14810 -5.372807 4.574058 0.036973 14910 -1.139746 5.196457 2.692685 15110 -1.810174 6.398177 -1.966035 15210 4.087479 5.351104 1.190975 15410 3.357942 4.244284 2.359336 15510 2.997312 4.269093 -3.308429 15610 3.908641 5.368534 -2.258782 15710 -4.994455 2.030936 -2.554888	135	1	0	6.5/0/63	2.011804	-0./86204
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	130	1	0	5.494525	4.210630	-0.623161
13810 5.670254 0.242336 2.270260 13910 4.776088 0.052444 -3.338158 14010 6.319567 0.067356 -2.471920 14110 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 0.092187 6.918541 -0.271712 14710 -3.443141 6.086282 -0.077071 14810 -5.372807 4.574058 0.036973 14910 -1.490460 6.550972 1.607243 15010 -1.518458 4.973960 -2.981107 15210 -1.810174 6.398177 -1.966035 15310 2.997312 4.269093 -3.308429 15410 3.357942 4.244284 2.359336 15510 3.908641 5.368534 -2.258782 15710 -4.994455 2.030936 -2.554888	137	1	0	0.80/884	0.238275	0.975585
13910 4.776088 0.052444 -3.338158 14010 6.319567 0.067356 -2.471920 14110 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 0.092187 6.918541 -0.271712 14710 -3.443141 6.086282 -0.077071 14810 -5.372807 4.574058 0.036973 14910 -1.490460 6.550972 1.607243 15010 -1.518458 4.973960 -2.981107 15210 -1.810174 6.398177 -1.966035 15310 3.357942 4.244284 2.359336 15510 2.997312 4.269093 -3.308429 15610 3.908641 5.368534 -2.258782 15710 -4.994455 2.030936 -2.554888	138	1	0	5.0/0254	0.242330	2.2/0200
14010 6.319367 0.067356 -2.471920 14110 3.734296 -3.938813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 0.092187 6.918541 -0.271712 14710 -3.443141 6.086282 -0.077071 14810 -5.372807 4.574058 0.036973 14910 -1.490460 6.550972 1.607243 15010 -1.518458 4.973960 -2.981107 15210 -1.810174 6.398177 -1.966035 15310 3.357942 4.244284 2.359336 15510 2.997312 4.269093 -3.308429 15610 3.908641 5.368534 -2.258782 15710 -4.994455 2.030936 -2.554888	140	1	0	4.770088	0.052444	-3.338158
14110 3.734296 -3.936813 2.694099 14210 4.455620 -5.055787 1.523026 14310 2.965119 -4.155047 -2.932689 14410 3.995715 -5.156041 -1.902432 14510 2.501869 6.466887 -0.387275 14610 0.092187 6.918541 -0.271712 14710 -3.443141 6.086282 -0.077071 14810 -5.372807 4.574058 0.036973 14910 -1.490460 6.550972 1.607243 15010 -1.518458 4.973960 -2.981107 15210 -1.810174 6.398177 -1.966035 15310 3.357942 4.244284 2.359336 15510 2.997312 4.269093 -3.308429 15610 3.908641 5.368534 -2.258782 15710 -4.994455 2.030936 -2.554888	140	1	0	0.319507	0.00/350	-2.4/1920
14210 4.435620 -5.035787 1.523026 143 10 2.965119 -4.155047 -2.932689 144 10 3.995715 -5.156041 -1.902432 145 10 2.501869 6.466887 -0.387275 146 10 0.092187 6.918541 -0.271712 147 10 -3.443141 6.086282 -0.077071 148 10 -5.372807 4.574058 0.036973 149 10 -1.490460 6.550972 1.607243 150 10 -1.518458 4.973960 -2.981107 152 10 -1.810174 6.398177 -1.966035 153 10 3.357942 4.244284 2.359336 155 10 2.997312 4.269093 -3.308429 156 10 3.908641 5.368534 -2.258782 157 10 -4.994455 2.030936 -2.554888	141 142	1	0	3.734290	-3.930013 E 0EE707	2.094099
14310 2.903119 -4.133047 -2.932089 144 10 3.995715 -5.156041 -1.902432 145 10 2.501869 6.466887 -0.387275 146 10 0.092187 6.918541 -0.271712 147 10 -3.443141 6.086282 -0.077071 148 10 -5.372807 4.574058 0.036973 149 10 -1.490460 6.550972 1.607243 150 10 -1.139746 5.196457 2.692685 151 10 -1.518458 4.973960 -2.981107 152 10 -1.810174 6.398177 -1.966035 153 10 3.357942 4.244284 2.359336 155 10 2.997312 4.269093 -3.308429 156 10 3.908641 5.368534 -2.258782 157 10 -4.994455 2.030936 -2.554888	142	1	0	4.455020		1.523020
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14510 2.501809 6.466887 -0.387275 146 10 0.092187 6.918541 -0.271712 147 10 -3.443141 6.086282 -0.077071 148 10 -5.372807 4.574058 0.036973 149 10 -1.490460 6.550972 1.607243 150 10 -1.139746 5.196457 2.692685 151 10 -1.518458 4.973960 -2.981107 152 10 -1.810174 6.398177 -1.966035 153 10 3.357942 4.244284 2.359336 155 10 2.997312 4.269093 -3.308429 156 10 3.908641 5.368534 -2.258782 157 10 -4.994455 2.030936 -2.554888	144	1	0	3.995/15	-5.150041	-1.902432
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	145	1	0	2.501009	0.40000/ 6 010E/1	-0.30/2/5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	140	1	0	2 112111	6 006202	-0.271712
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	140	1	0	- 3.443141 E 272007	0.000202	0.026072
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	140	1	0	-5.572807	4.574058 6 550072	1 607242
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	150	1	0	-1.490400 -1.1307/6	5 196457	2 602685
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	151	1	0	-1 518458	4 973960	-2 981107
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	152	⊥ 1	0	_1 81017 <i>4</i>		-1 966035
153 1 0 4.067479 5.351104 1.190975 154 1 0 3.357942 4.244284 2.359336 155 1 0 2.997312 4.269093 -3.308429 156 1 0 3.908641 5.368534 -2.258782 157 1 0 -4.994455 2.030936 -2.554888	153	⊥ 1	0	1 007/70	5 35110/	1 100075
151 1 0 3.337942 4.244264 2.359336 155 1 0 2.997312 4.269093 -3.308429 156 1 0 3.908641 5.368534 -2.258782 157 1 0 -4.994455 2.030936 -2.554888	154	⊥ 1	0	7,00/4/9	Δ ΟΔΔΟΩΛ	7 320336
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	155	⊥ 1	0) QQ7210	1.211204 2 960002	-3 3U8NJ0 000007
157 1 0 -4.994455 2.030936 -2.554888	156	⊥ 1	0	2.997312 2 909641		-2 258782
	157	1	0	-4.994455	2.030936	-2.554888

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Z
158	1	0	-6.208757	2.718062	-1.465321
159	1	0	-4.880040	2.563963	3.099594
160	1	0	-6.166581	3.015057	1.967280
161	1	0	-5.131800	-2.598309	-2.195101
162	1	0	-6.210020	-3.098076	-0.883510
163	1	0	-4.312136	-1.940504	3.397832
164	1	0	-5.681288	-2.722917	2.588740
165	1	0	-6.815900	-1.283463	0.780485
166	1	0	-6.940397	1.142613	0.439880

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