

## **Supporting Information**

**for**

# **Calix[6]arene-based atropoisomeric pseudo[2]rotaxanes**

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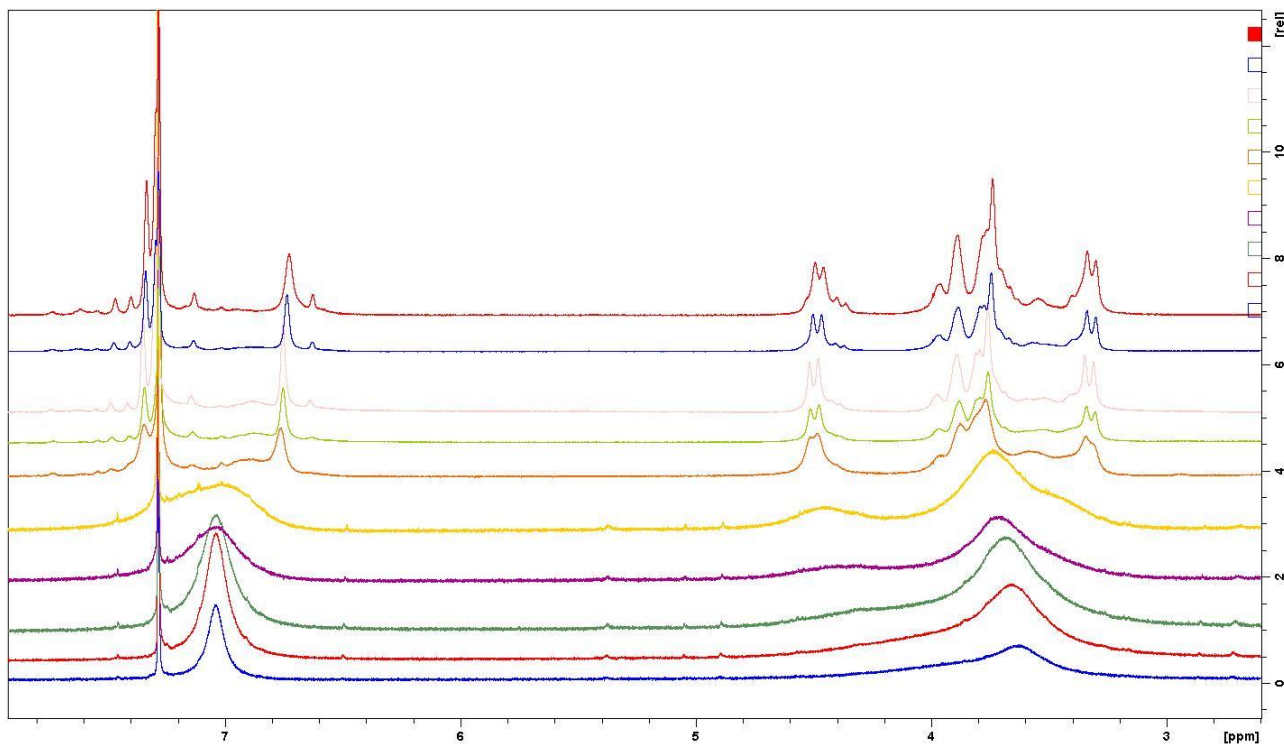
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\*Corresponding author

**VT NMR studies of hexyloxy-calix[6]arene 1, 2D COSY and HSQC spectra  
of atropoisomeric pseudorotaxanes, details of DFT calculations and  
atomic coordinates**

## Variable Temperature $^1\text{H}$ NMR Spectra of **1** ( $\text{CDCl}_3$ , 600 MHz)



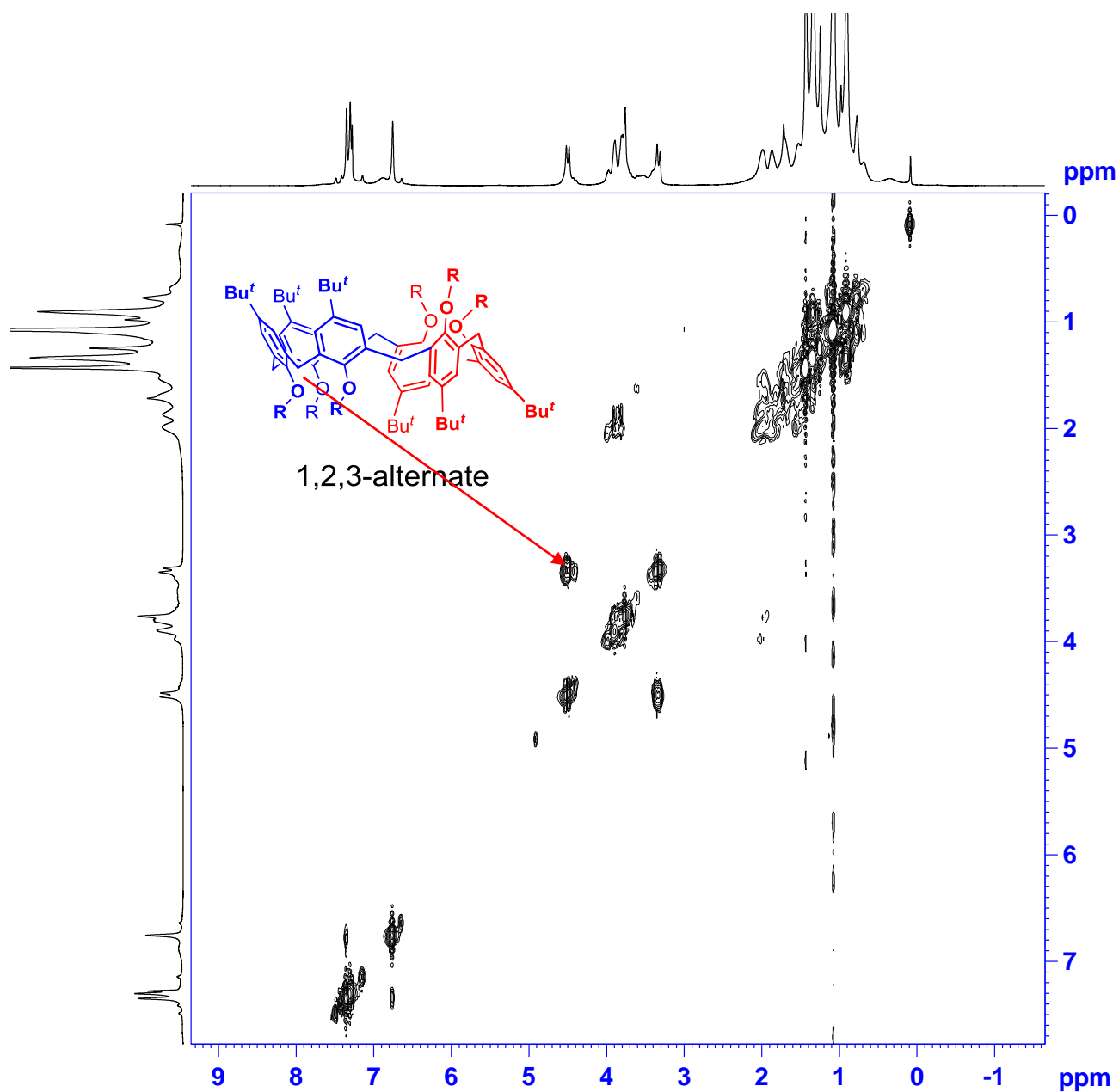
**Figure S1:**  $^1\text{H}$  NMR spectra of **1** (400 MHz,  $\text{CDCl}_3$ ) at (from bottom to top): **328** ( $T_c$ ); 323; 318; 313; 298; 273; 263; 253; 243; 233 K.

$$\Delta G_c^\ddagger = aT_c \left[ 9.972 + \log \left( \frac{T_c}{\sqrt{\Delta \nu^2 + 6J^2}} \right) \right]$$

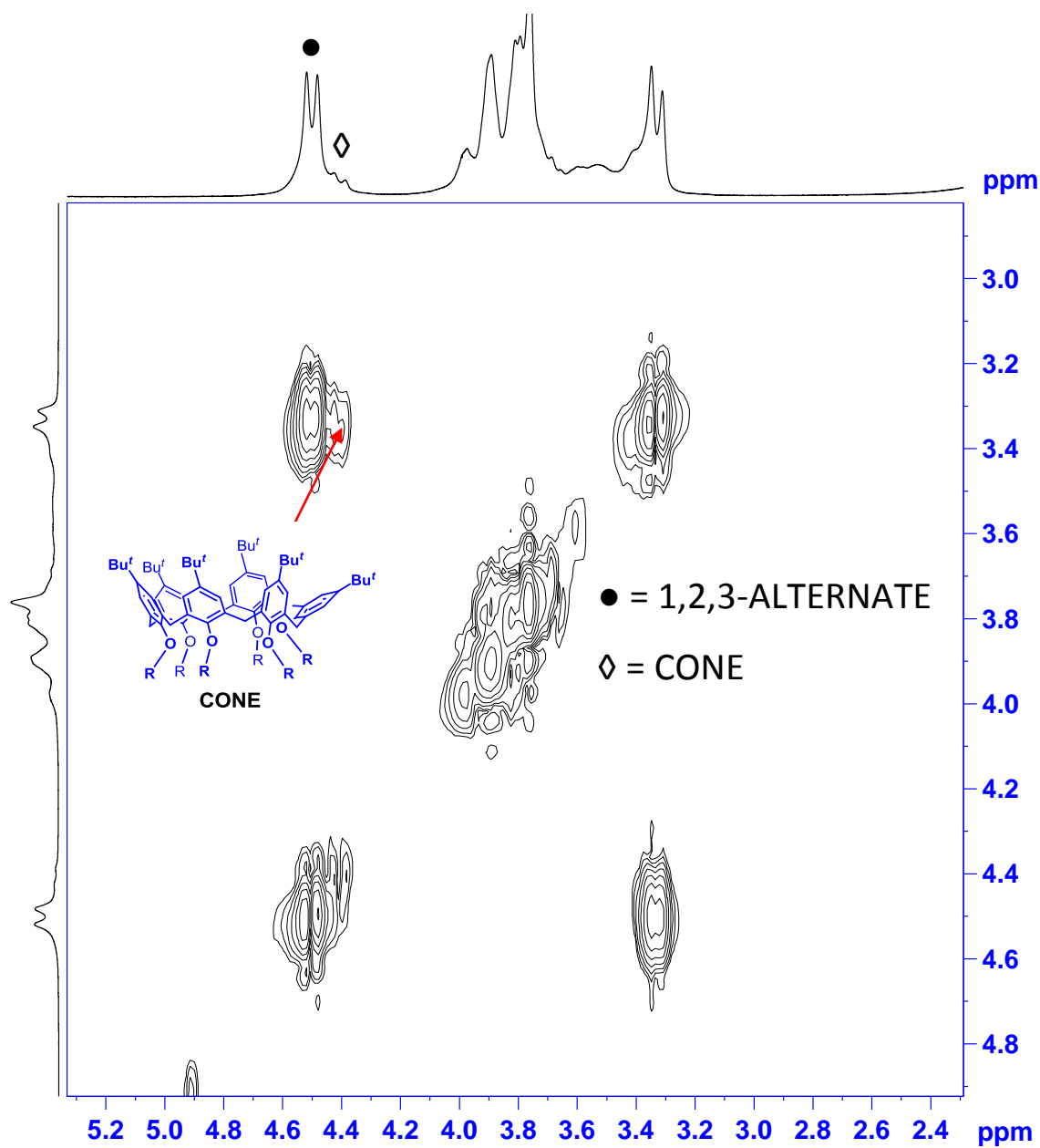
Kurland, R. J.; Rubin, M. B.; Wise, M. B. *J. Chem. Phys.* **1964**, *40*, 2426

$T_c = 328$  K;  $\Delta \nu = 466$  Hz ;  $a = 4.575 \cdot 10^{-3}$  ( $\Delta G_c^\ddagger$  in Kcal/mol)

## 2D Spectra of 1 at 233 K (CDCl<sub>3</sub>, 600 MHz)



**Figure S2:** COSY spectrum of **1** (600 MHz, CDCl<sub>3</sub>) at 233 K.



**Figure S3:** Expansion of the COSY spectrum of **1** (600 MHz, CDCl<sub>3</sub>) at 233 K.

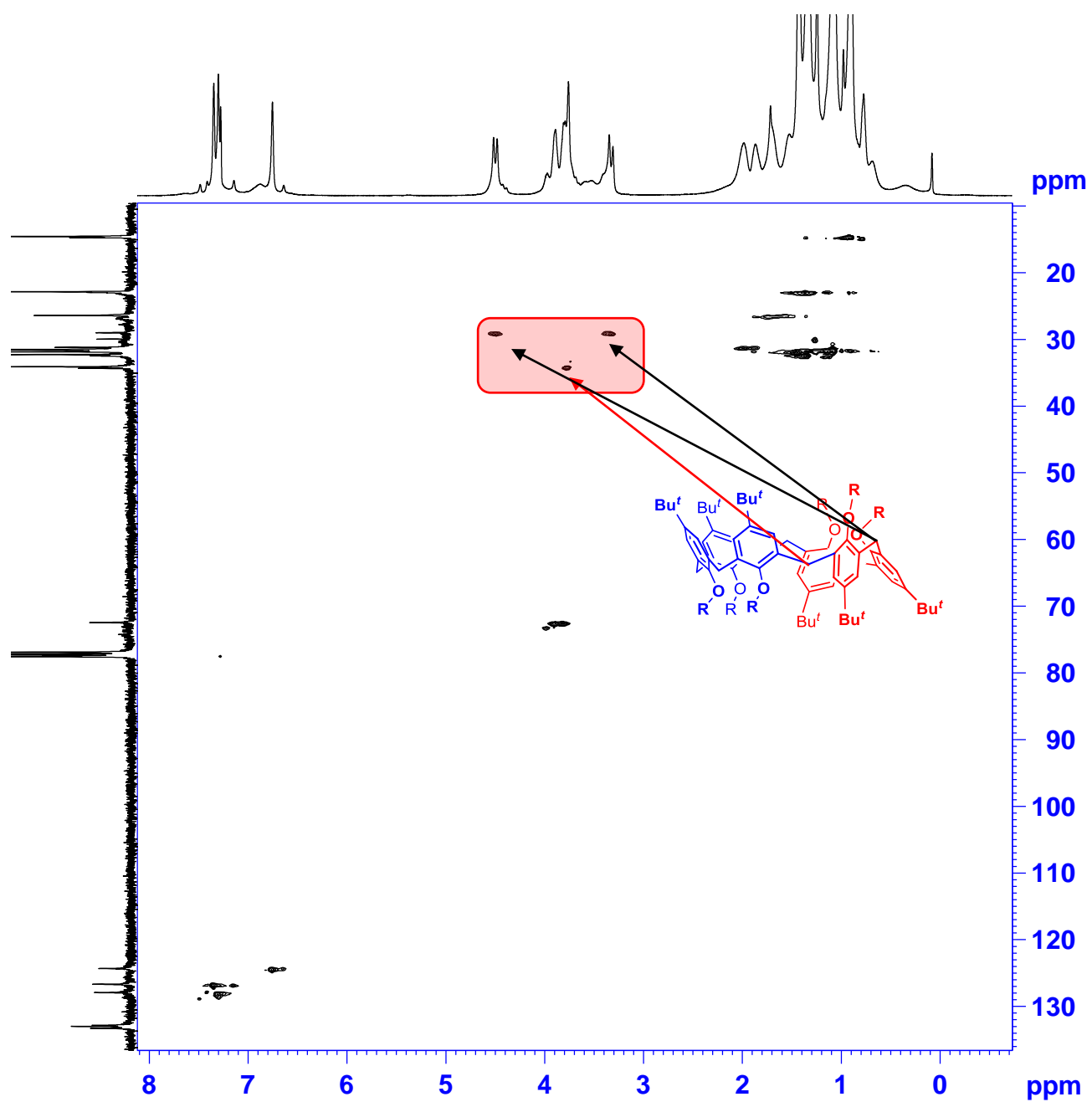
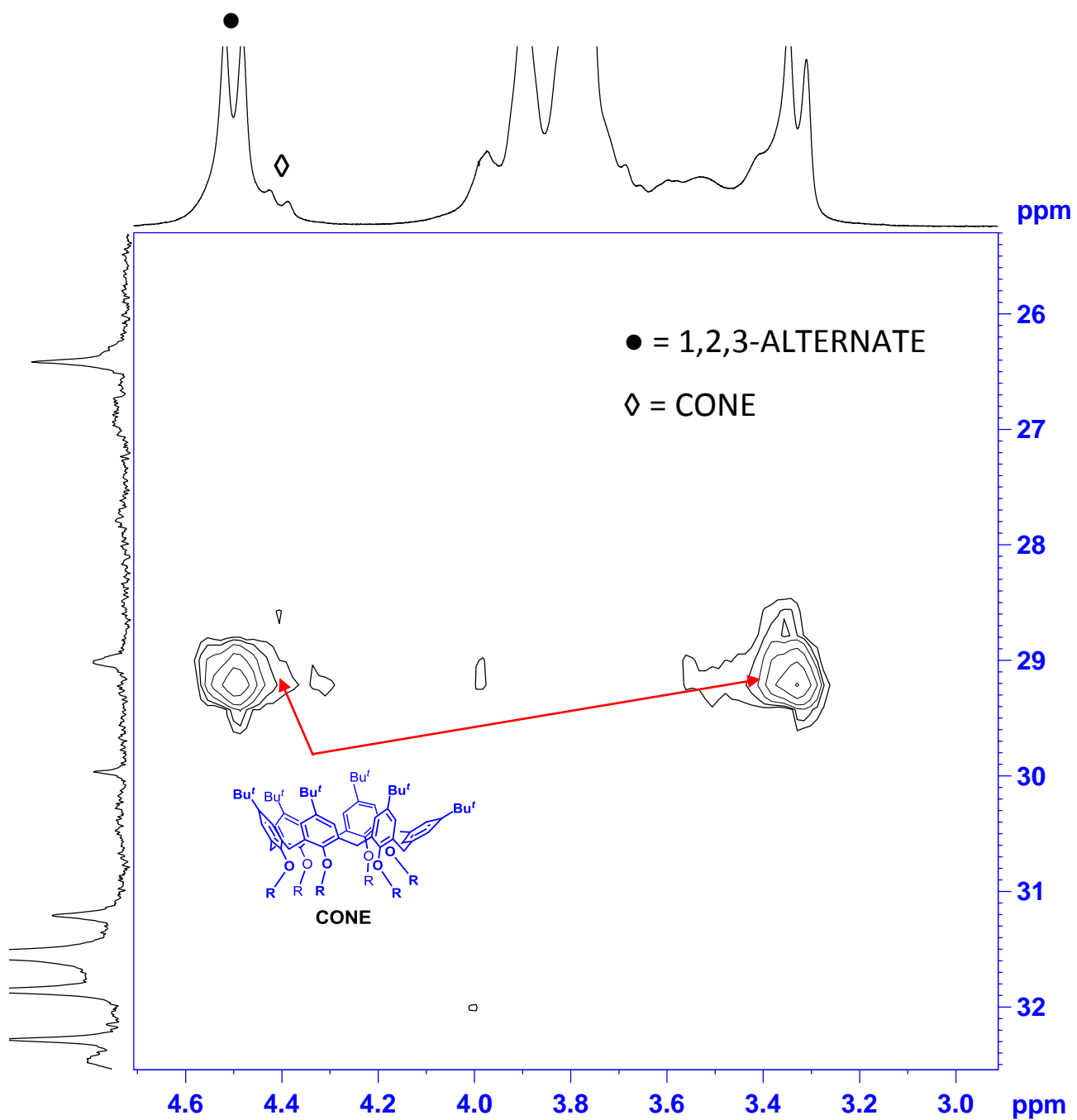
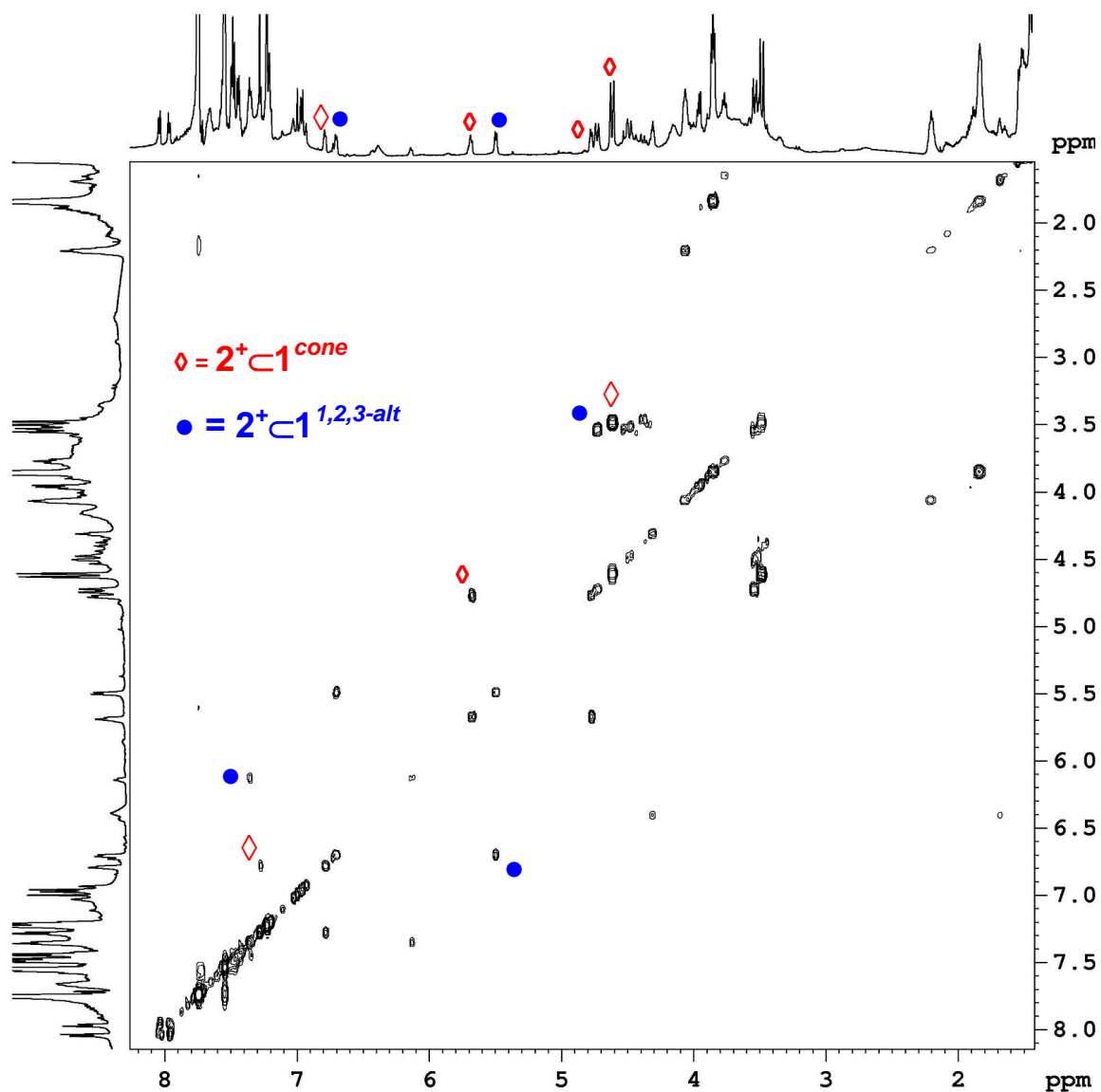


Figure S4: HSQC spectrum of 1 (600 MHz,  $\text{CDCl}_3$ ) at 233 K.



**Figure S5:** Expansion of the HSQC spectrum of **1** (600 MHz, CDCl<sub>3</sub>) at 233 K.

2D COSY spectrum of  $2^+ \subset 1^{cone}$  and  $2^+ \subset 1^{1,2,3-alt}$  atropoisomers at 298 K  
( $CDCl_3$ , 600 MHz)



**Figure S6:** COSY spectrum (600 MHz,  $CDCl_3$ , 298 K) of a 1:1 mixture (0.003 M) of **1** and  $2^+ \cdot TFPB^-$  after 10 h by mixing.

2D COSY spectrum of  $2^+ \subset 1^{cone}$  atropoisomer at 298 K ( $CDCl_3$ , 600 MHz)

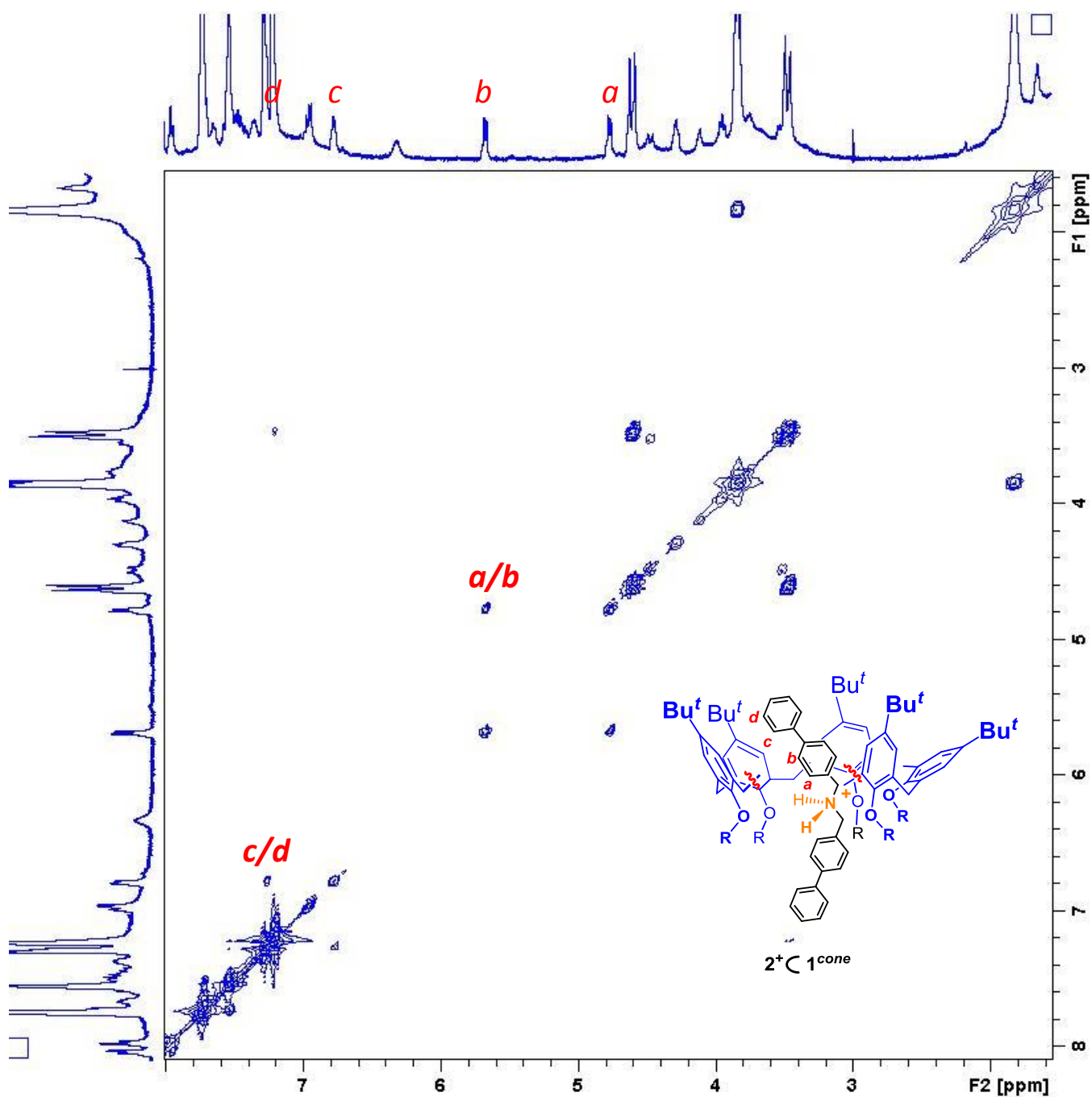


Figure S7: COSY spectrum (600 MHz,  $CDCl_3$ , 298 K) of a 1:1 mixture (0.003 M) of **1** and  $2^+ \cdot TFPB^-$  after 18 h by mixing,  $2^+ \subset 1^{cone}$ .



2D HSQC spectrum of  $2^+ \subset 1^{cone}$  atropoisomer at 298 K ( $CDCl_3$ , 600 MHz)

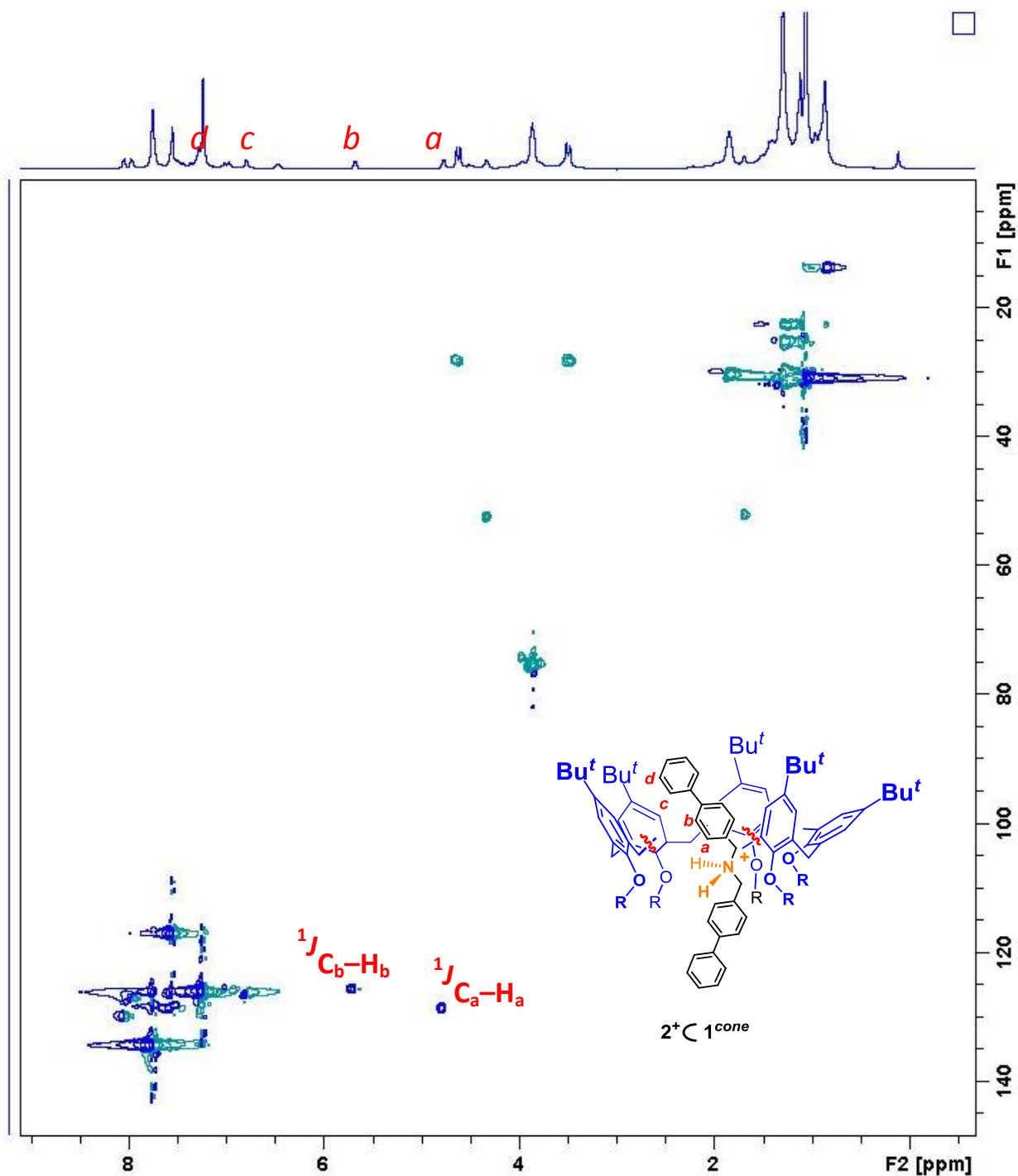
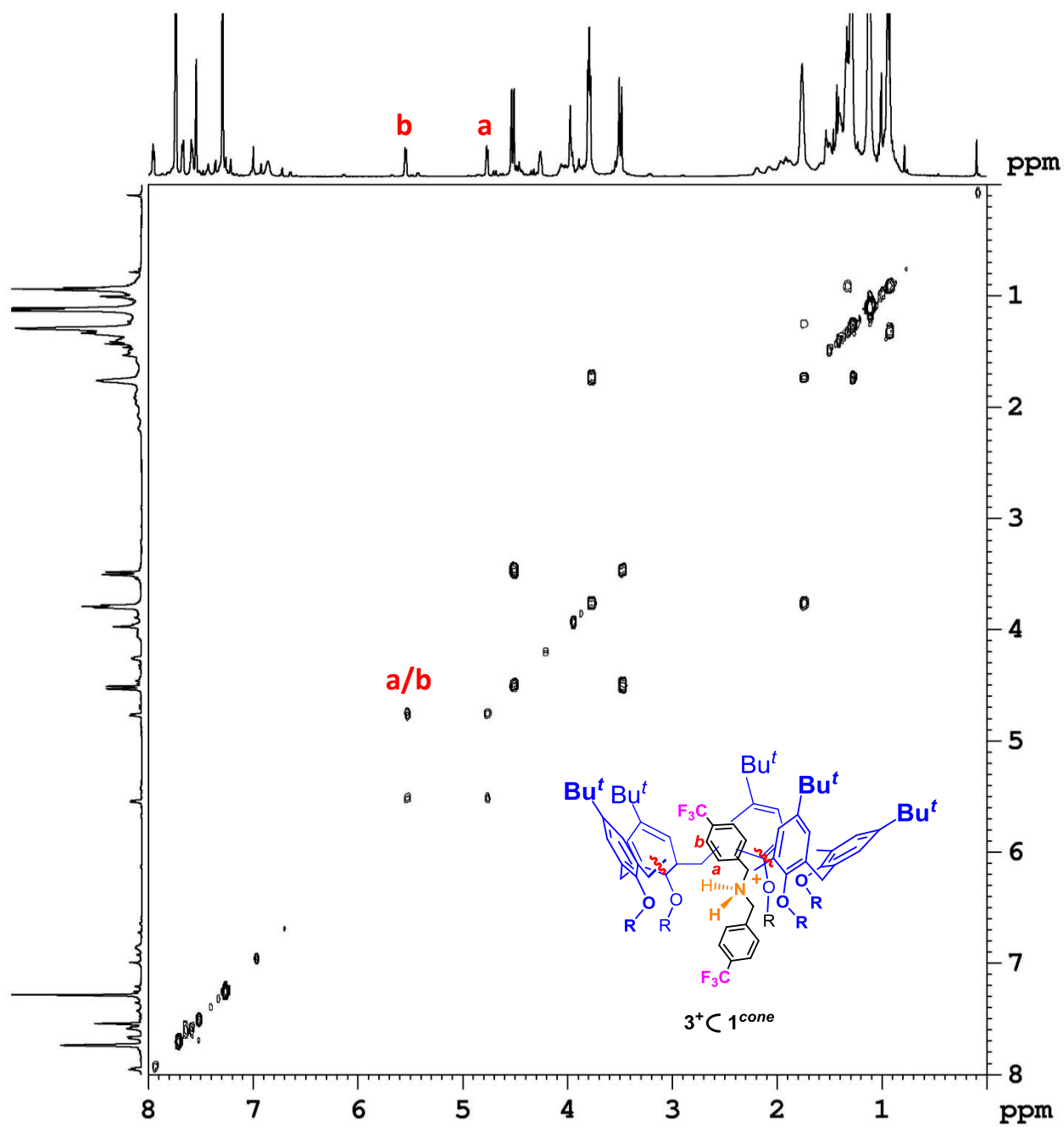
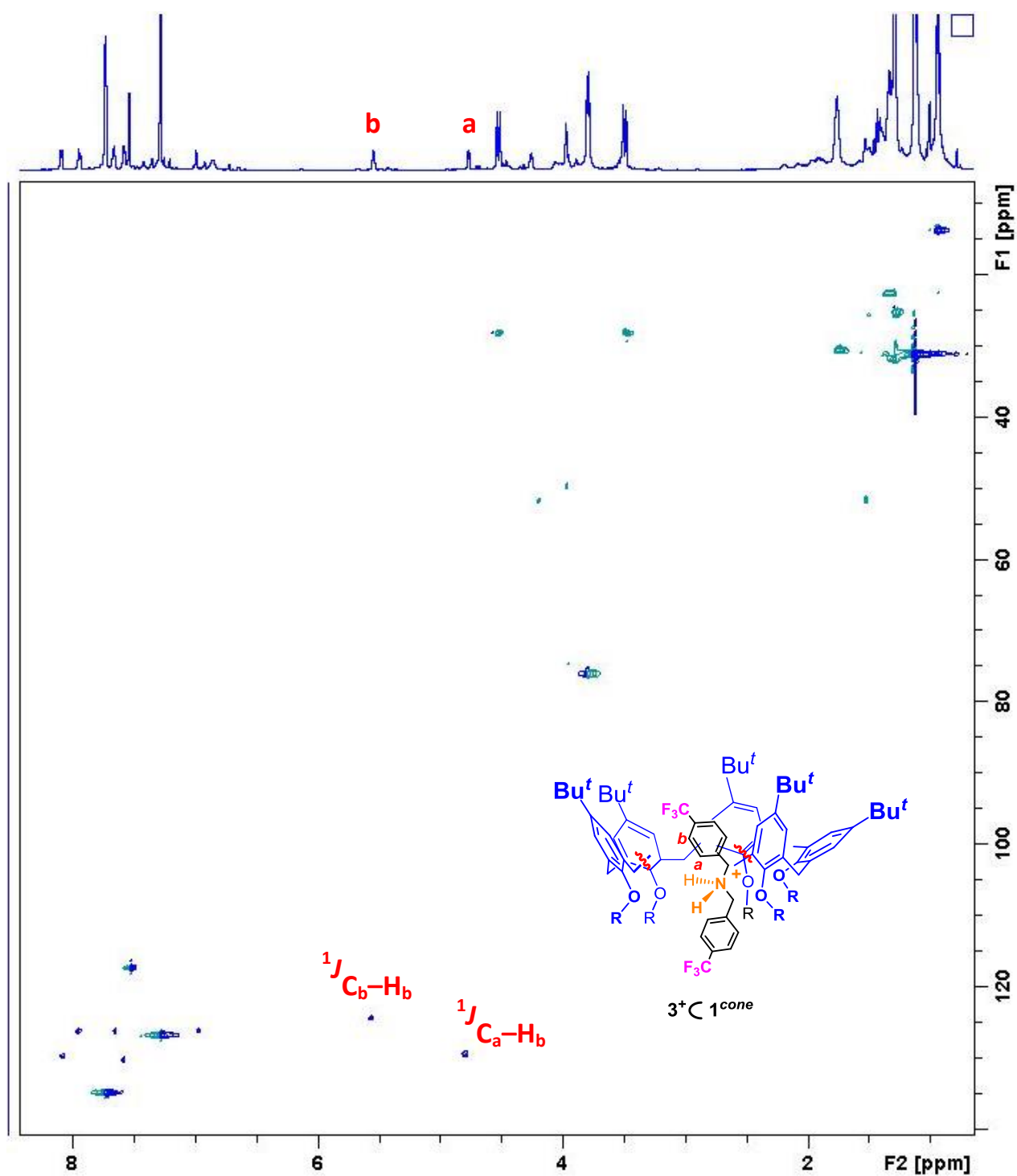


Figure S8: HSQC spectrum (600 MHz,  $CDCl_3$ , 298 K) of a 1:1 mixture (0.003 M) of **1** and  $2^+ \cdot TFPB^-$  after 18 h by mixing,  $2^+ \subset 1^{cone}$ .

2D COSY spectrum of  $3^+ \subset 1^{cone}$  atropisomer at 298 K ( $CDCl_3$ , 600 MHz)





**Figure S10:** HSQC spectrum (600 MHz,  $\text{CDCl}_3$ , 298 K) of a 1:1 mixture (0.003 M) of **1** and  $3^+\cdot\text{TFPB}^-$  after 24 h,  $3^+ \text{C } 1^{\text{cone}}$ .

**Determination of apparent association constant values by quantitative  $^1\text{H}$  NMR analysis (for pseudorotaxanes  $2^+\subset 1^{\text{cone}}$ ,  $3^+\subset 1^{\text{cone}}$  and  $3^+\subset 1^{1,2,3\text{-alt}}$ ).**

The samples were prepared by dissolving calixarene-1 ( $3.0 \times 10^{-3}$  M) and the appropriate ammonium TFPB salt ( $2^+$  or  $3^+$ ) ( $3.0 \times 10^{-3}$  M) in  $\text{CDCl}_3$  (0.5 mL) containing 0.10  $\mu\text{L}$  of TCHE ( $d = 1.596$  g/mL) as an internal standard. The complex concentration [complex] was evaluated by integration of the  $^1\text{H}$  NMR signals of TCHE versus the signals of the pseudorotaxane. The following equation was used to obtain the moles of the complex:

$$\frac{G_a}{G_b} = \frac{F_a}{F_b} \times \frac{N_b}{N_a} \times \frac{M_a}{M_b}$$

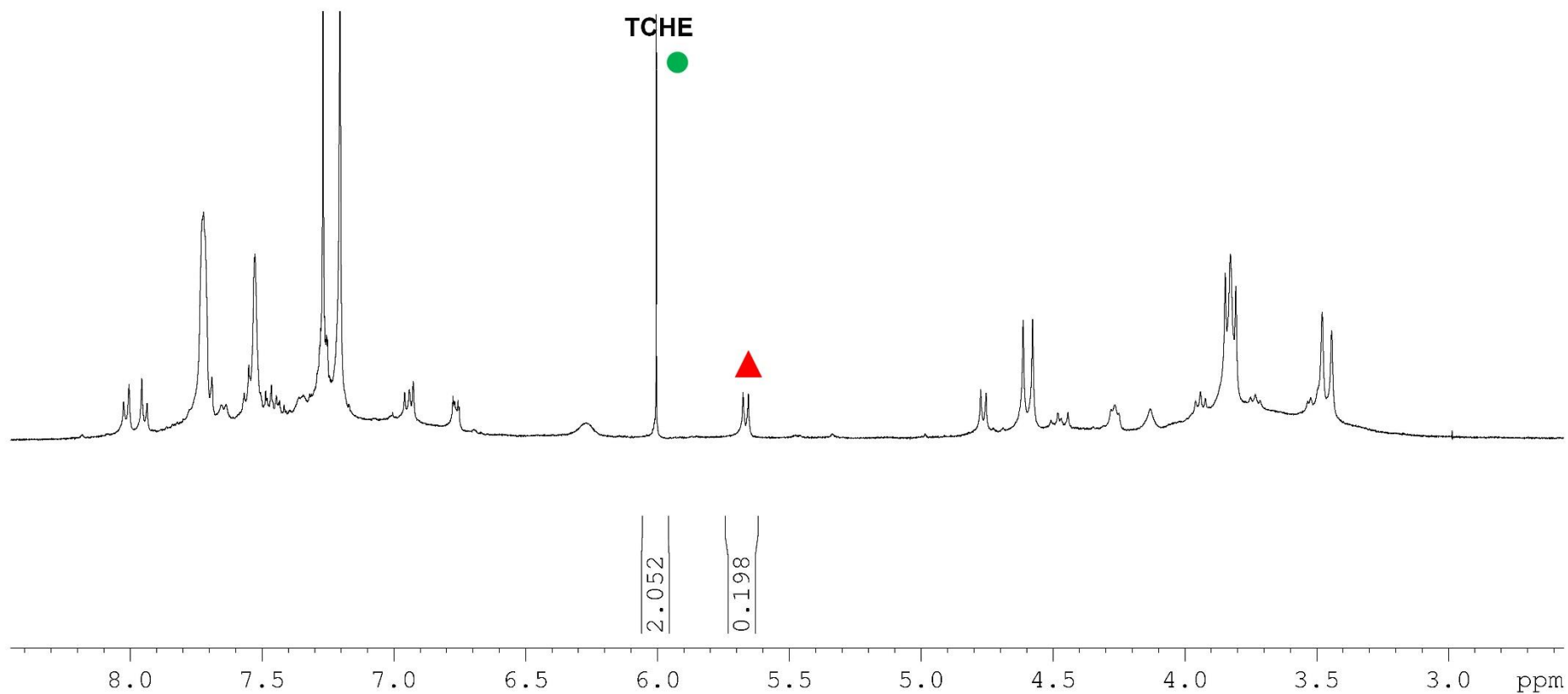
in which:

$G_a$  = grams of TCHE;  $G_b$  = grams of pseudorotaxane

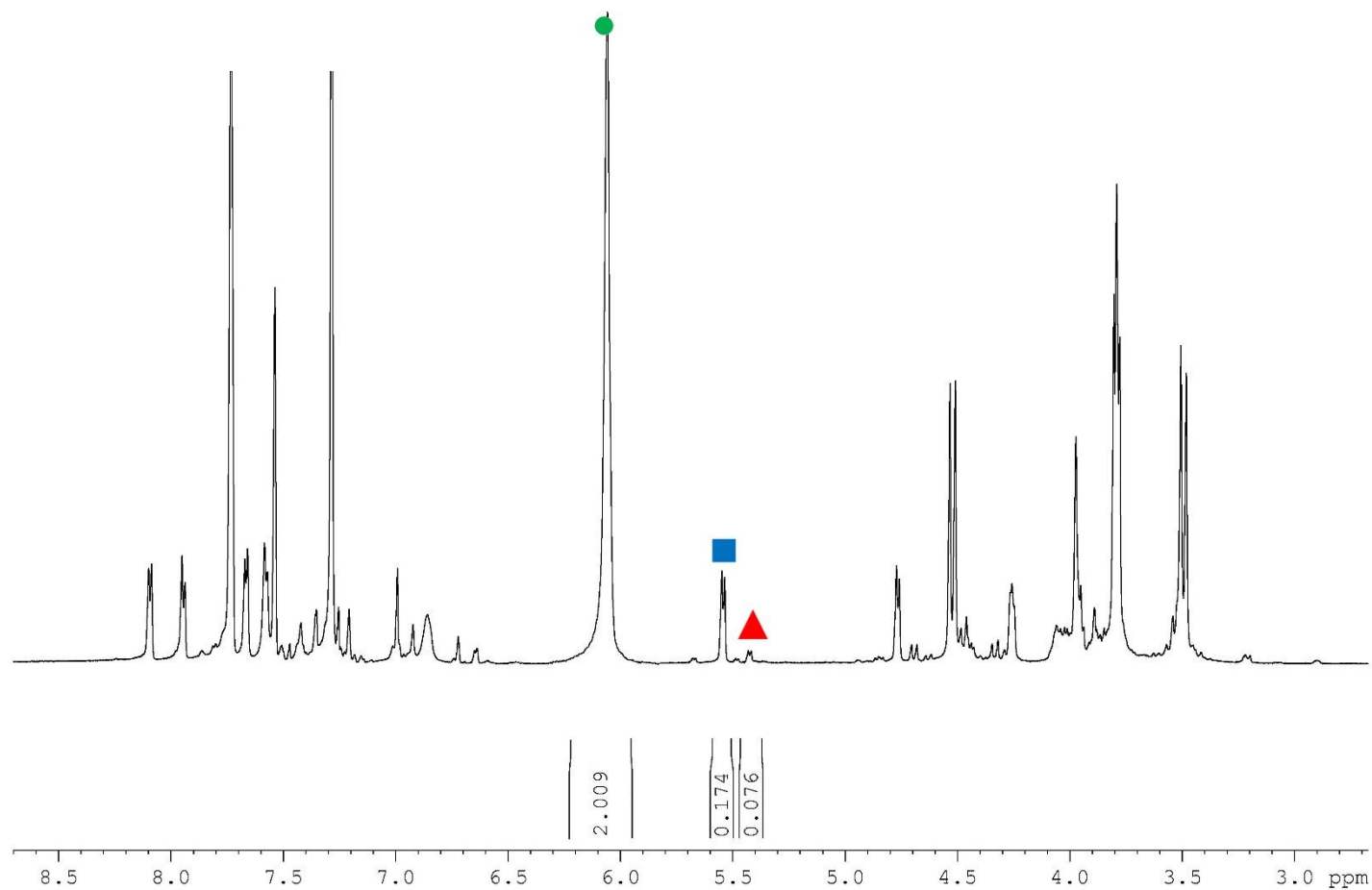
$F_a$  and  $F_b$  = areas of the signals of, TCHE and shielded aromatic protons of the axle.

$N_a$  and  $N_b$  = are the numbers of nuclei that cause the signals ( $N_a$  for TCHE;  $N_b$  for pseudorotaxane)

$M_a$  and  $M_b$  = are the molecular masses of TCHE (a) and pseudorotaxane (b)



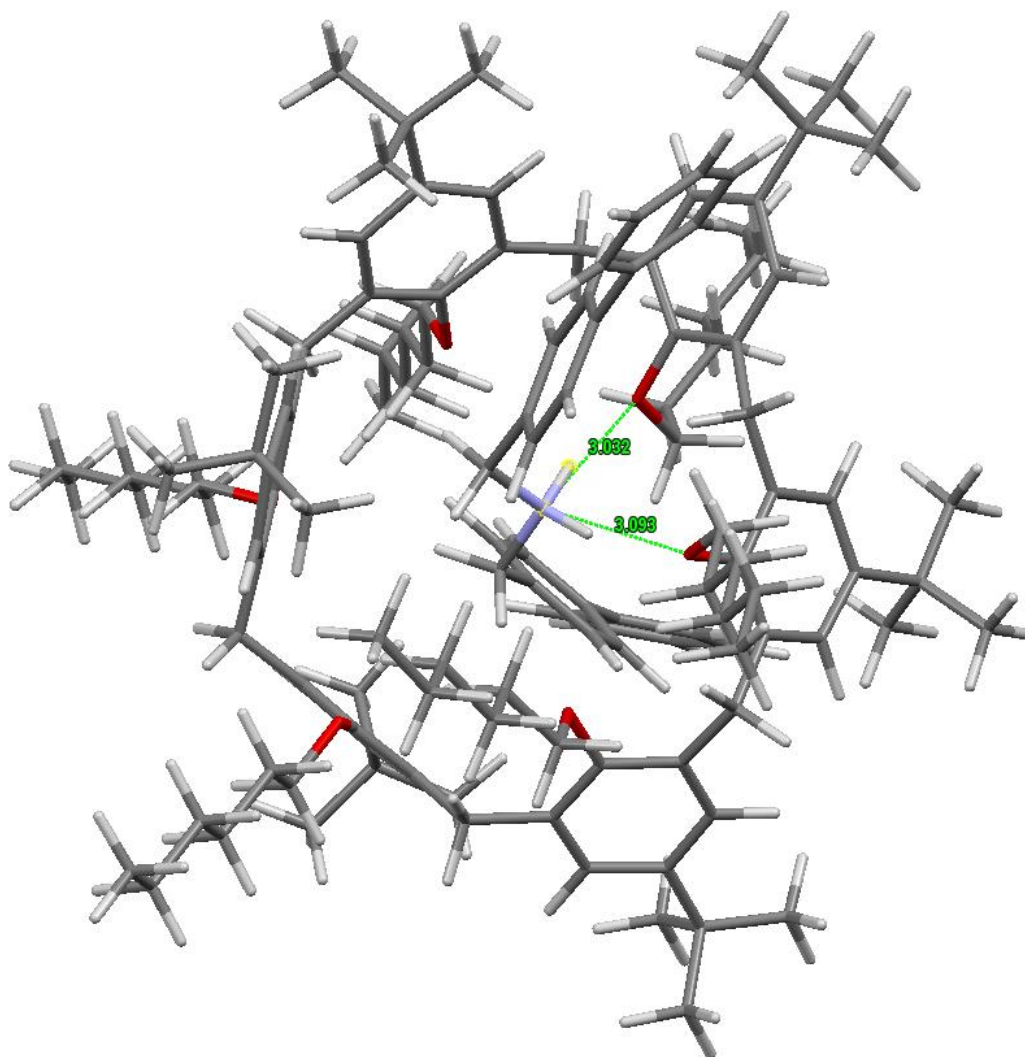
**Figure S11.** <sup>1</sup>H NMR spectra (600 MHz, CDCl<sub>3</sub>, 298 K) of a 1:1 mixture (0.003 M) of hexahexyloxycalix[6]arene **1** and **2<sup>+</sup>·TFPB<sup>-</sup>** in 0.5 mL of CDCl<sub>3</sub> containing 1.0 μL of TCHE after equilibration for 48 h at 298 K. The association constant  $K_a$  values were calculated by integration of complexed ArH signal of **2<sup>+</sup>·1<sup>cone</sup>** (▲) and signal of TCHE (●).



**Figure S12.**  $^1\text{H}$  NMR spectra (600 MHz,  $\text{CDCl}_3$ , 298 K) of a 1:1 mixture (0.0024 M) of hexahexyloxycalix[6]arene **1** and  $2^+\cdot\text{TFPB}^-$  in 0.5 mL of  $\text{CDCl}_3$  containing 0.10  $\mu\text{L}$  of TCHE after equilibration for 48 h at 298 K. The association constant  $K_a$  values were calculated by integration of complexed  $\text{ArH}$  signals of  $3^+\subset 1^{\text{cone}}$  (■),  $3^+\subset 1^{1,2,3\text{-alt}}$  (▲) and signal of TCHE (●).

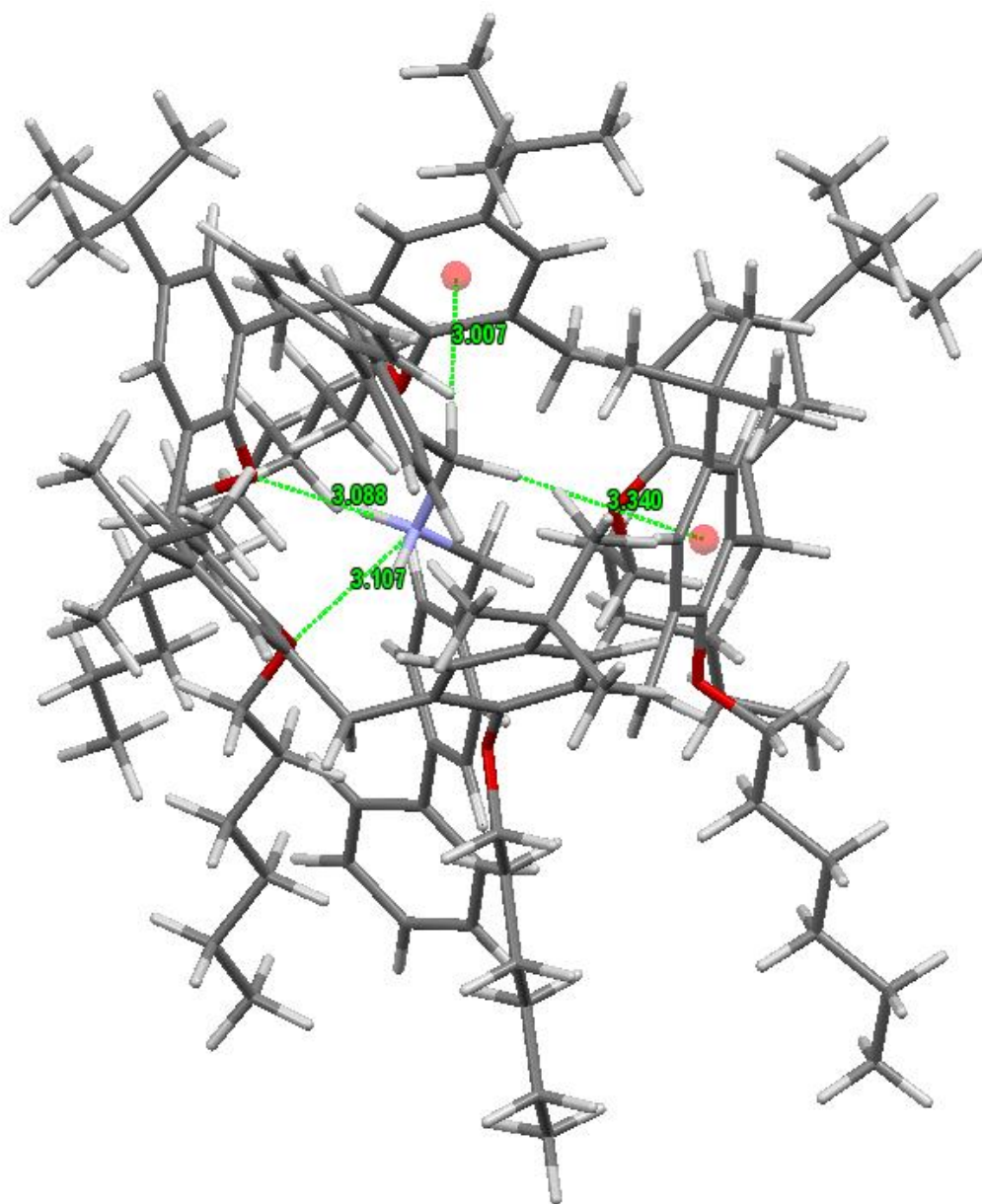
## DFT Calculations.

Preliminary conformational searches have been performed by molecular mechanics calculations (Spartan 02). The minimized structures were optimized by DFT calculations (Gaussian 09) at B3LYP/6-31G(d,p) level of theory using Grimme's dispersion corrections



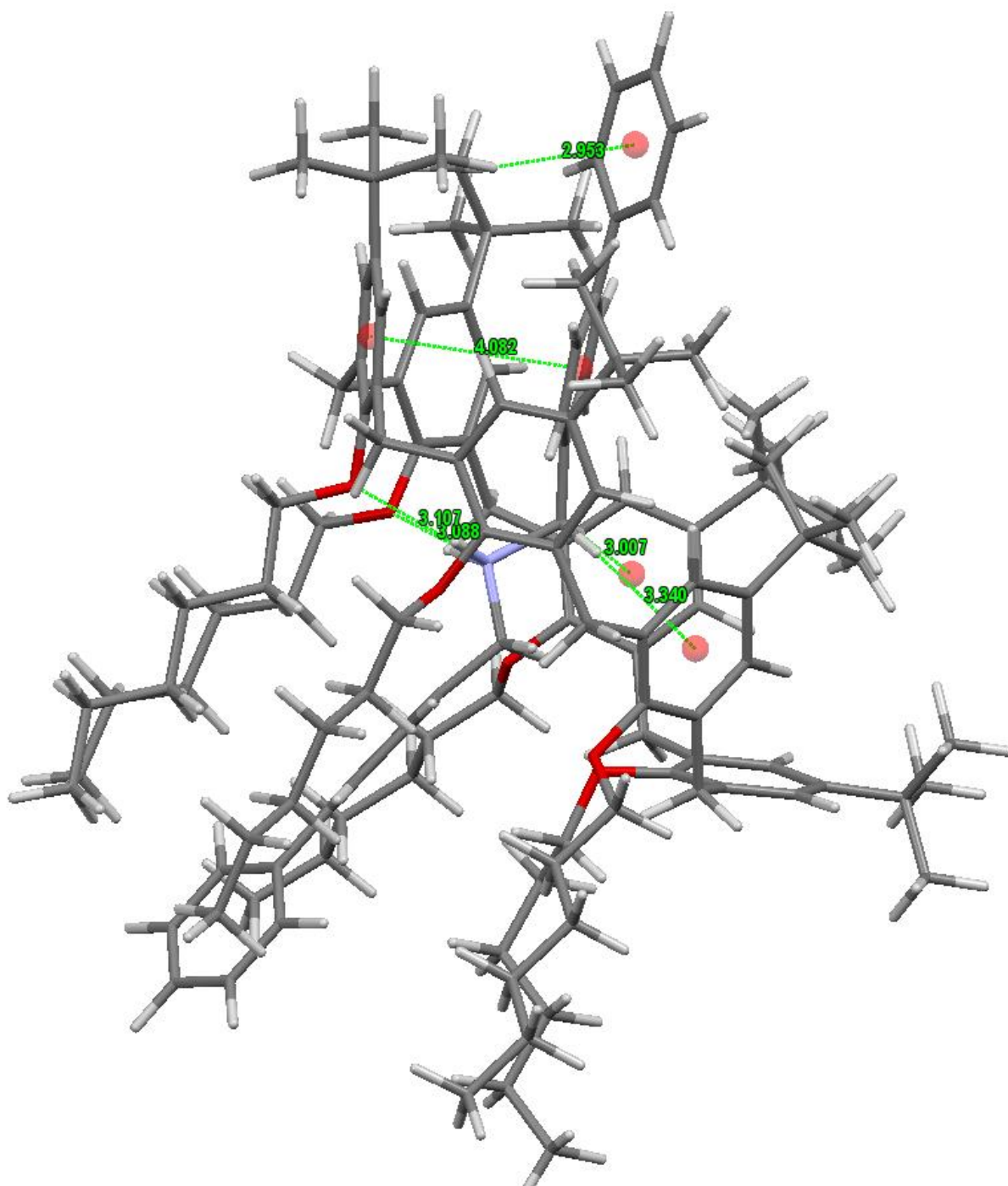
(IOp(3/124 = 3)).

**Figure S13:** DFT-optimized structure of the  $2^+ \text{C}1^{\text{cone}}$  atropisomer with H-bonds N...O distances indicated.

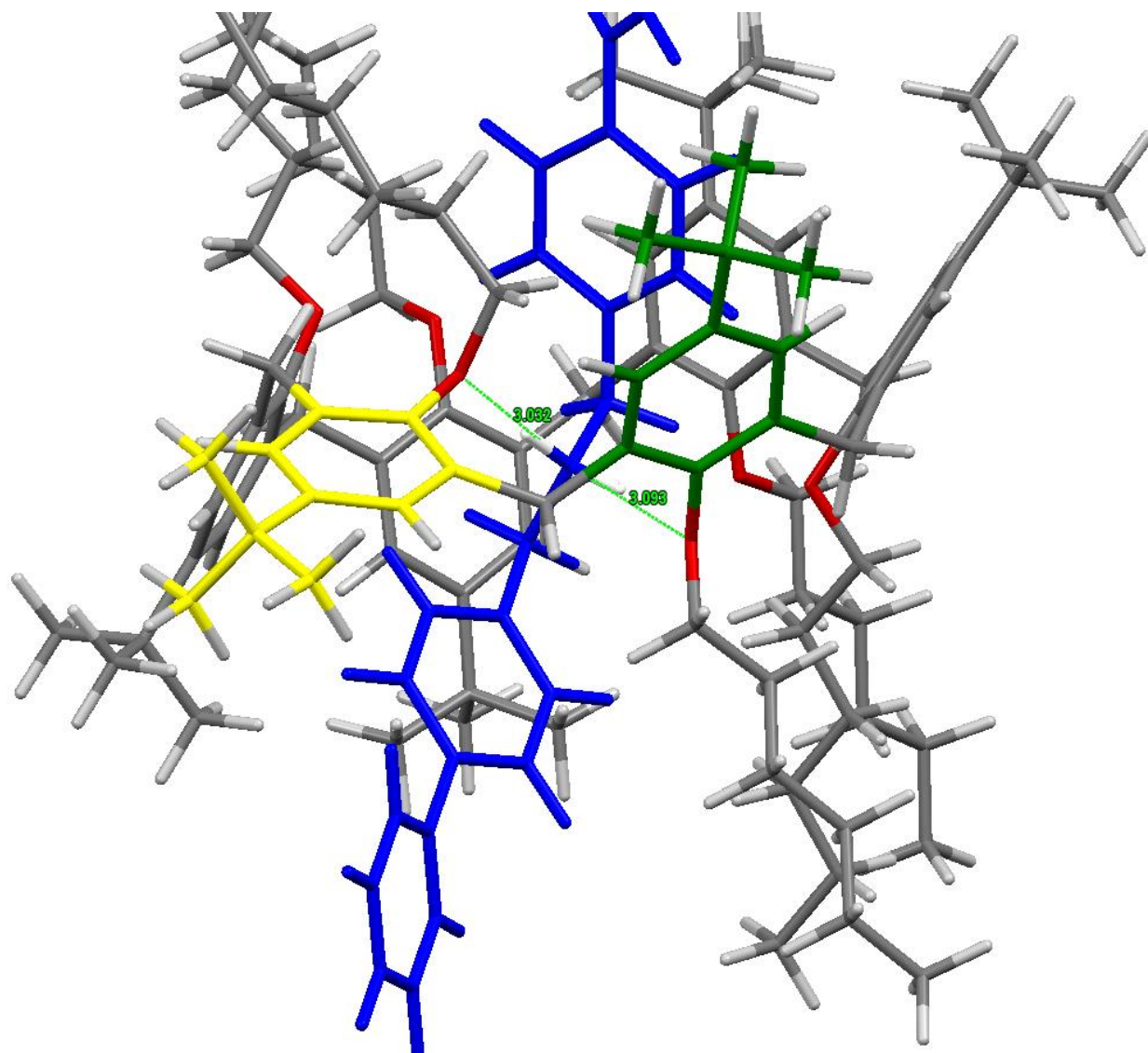


**Figure S14:** DFT-optimized structure of the  $2^+ \subset 1^{cone}$  atropisomer with C-H... $\pi$  distances indicated.

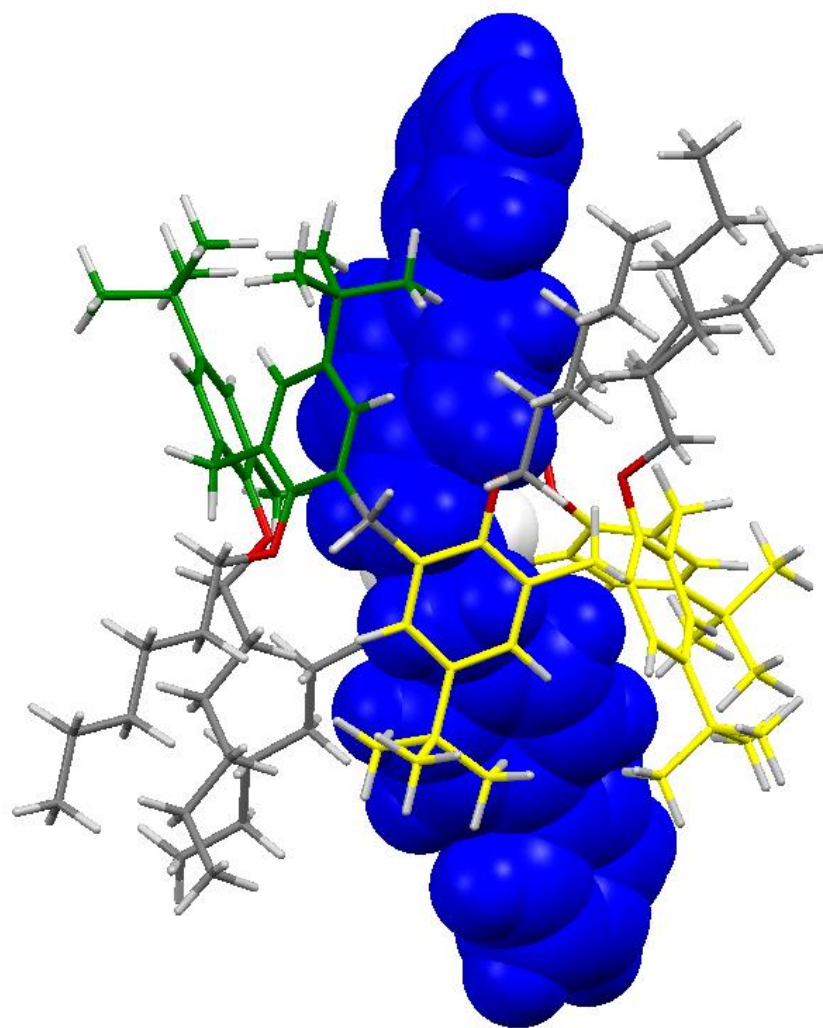




**Figure S15:** DFT-optimized structure of the  $2^+ \text{C1}^{\text{cone}}$  atropisomer with C-H... $\pi$  and  $\pi$ ... $\pi$  distances indicated.



**Figure S16:** DFT-optimized structure of the  $2^+ C_1^{1,2,3-alt}$  atropisomer with H-bonds N...O distances indicated.



**Figure S17:** Different view of the DFT-optimized structure of the  $2^+ \subset 1^{1,2,3-alt}$  atropisomer.

## Atomic coordinates of $2^+ \subset 1^{cone}$

HETATM	1	O1	UNK	1	0.141	4.032	-0.402	1.00	0.00	O
HETATM	2	O2	UNK	1	-2.211	2.787	2.878	1.00	0.00	O
HETATM	3	O3	UNK	1	-1.376	-4.335	-0.395	1.00	0.00	O
HETATM	4	O4	UNK	1	-2.721	-1.382	2.257	1.00	0.00	O
HETATM	5	O5	UNK	1	0.881	-2.257	-2.796	1.00	0.00	O
HETATM	6	C6	UNK	1	-2.446	-1.914	3.508	1.00	0.00	C
HETATM	7	C7	UNK	1	1.273	1.248	4.666	1.00	0.00	C
HETATM	8	C8	UNK	1	-1.063	2.288	3.479	1.00	0.00	C
HETATM	9	C9	UNK	1	0.034	0.622	4.834	1.00	0.00	C
HETATM	10	C10	UNK	1	1.312	2.393	3.856	1.00	0.00	C
HETATM	11	C11	UNK	1	-2.420	-1.070	4.635	1.00	0.00	C
HETATM	12	C12	UNK	1	-2.014	-4.169	2.406	1.00	0.00	C
HETATM	13	C13	UNK	1	2.196	-2.720	-2.657	1.00	0.00	C
HETATM	14	C14	UNK	1	0.985	-4.628	0.024	1.00	0.00	C
HETATM	15	C15	UNK	1	-2.491	0.441	4.500	1.00	0.00	C
HETATM	16	C16	UNK	1	-0.325	-4.438	0.510	1.00	0.00	C
HETATM	17	C17	UNK	1	-2.250	-1.653	5.893	1.00	0.00	C
HETATM	18	C18	UNK	1	3.738	4.723	0.028	1.00	0.00	C
HETATM	19	C19	UNK	1	-0.581	-4.338	1.890	1.00	0.00	C
HETATM	20	C20	UNK	1	1.435	4.453	1.590	1.00	0.00	C
HETATM	21	C21	UNK	1	3.817	5.028	1.389	1.00	0.00	C
HETATM	22	C22	UNK	1	2.982	-0.658	-3.929	1.00	0.00	C
HETATM	23	C23	UNK	1	-1.141	1.118	4.255	1.00	0.00	C
HETATM	24	C24	UNK	1	0.213	4.246	2.466	1.00	0.00	C
HETATM	25	C25	UNK	1	1.804	-4.714	2.339	1.00	0.00	C
HETATM	26	C26	UNK	1	1.246	-4.781	-1.475	1.00	0.00	C
HETATM	27	C27	UNK	1	0.497	-4.471	2.774	1.00	0.00	C
HETATM	28	C28	UNK	1	0.170	2.936	3.262	1.00	0.00	C
HETATM	29	C29	UNK	1	3.701	-4.488	-2.049	1.00	0.00	C
HETATM	30	C30	UNK	1	2.538	4.342	-0.595	1.00	0.00	C
HETATM	31	C31	UNK	1	4.540	-2.533	-3.146	1.00	0.00	C
HETATM	32	C32	UNK	1	-2.163	-3.282	3.629	1.00	0.00	C
HETATM	33	C33	UNK	1	3.256	-1.969	-3.189	1.00	0.00	C
HETATM	34	C34	UNK	1	4.790	-3.800	-2.608	1.00	0.00	C
HETATM	35	C35	UNK	1	2.402	-3.973	-2.049	1.00	0.00	C
HETATM	36	C36	UNK	1	1.380	4.257	0.194	1.00	0.00	C
HETATM	37	C37	UNK	1	2.021	-4.765	0.954	1.00	0.00	C
HETATM	38	C38	UNK	1	-2.062	-3.033	6.072	1.00	0.00	C
HETATM	39	C39	UNK	1	-1.996	-3.817	4.916	1.00	0.00	C
HETATM	40	C40	UNK	1	2.648	4.864	2.149	1.00	0.00	C
HETATM	41	C41	UNK	1	2.491	4.090	-2.102	1.00	0.00	C
HETATM	42	C42	UNK	1	4.726	3.143	-2.846	1.00	0.00	C
HETATM	43	C43	UNK	1	5.563	2.141	-3.361	1.00	0.00	C
HETATM	44	C44	UNK	1	4.980	0.900	-3.633	1.00	0.00	C
HETATM	45	C45	UNK	1	3.613	0.648	-3.447	1.00	0.00	C
HETATM	46	C46	UNK	1	2.814	1.693	-2.954	1.00	0.00	C
HETATM	47	C47	UNK	1	3.361	2.947	-2.620	1.00	0.00	C
HETATM	48	O48	UNK	1	1.427	1.522	-2.864	1.00	0.00	O
HETATM	49	C49	UNK	1	0.322	-2.701	-4.064	1.00	0.00	C
HETATM	50	H50	UNK	1	-0.041	-0.277	5.432	1.00	0.00	H
HETATM	51	H51	UNK	1	2.261	2.888	3.689	1.00	0.00	H
HETATM	52	H52	UNK	1	-2.621	-3.781	1.590	1.00	0.00	H
HETATM	53	H53	UNK	1	-2.407	-5.165	2.651	1.00	0.00	H
HETATM	54	H54	UNK	1	-2.921	0.848	5.425	1.00	0.00	H
HETATM	55	H55	UNK	1	-3.160	0.741	3.693	1.00	0.00	H

HETATM	56	H56	UNK	1	-4.104	-0.287	1.249	1.00	0.00	H
HETATM	57	H57	UNK	1	4.622	4.811	-0.590	1.00	0.00	H
HETATM	58	H58	UNK	1	0.157	5.077	3.183	1.00	0.00	H
HETATM	59	H59	UNK	1	-0.690	4.292	1.859	1.00	0.00	H
HETATM	60	H60	UNK	1	-2.474	-5.982	0.262	1.00	0.00	H
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HETATM	63	H63	UNK	1	3.023	-4.943	0.578	1.00	0.00	H
HETATM	64	H64	UNK	1	-1.829	-4.885	4.998	1.00	0.00	H
HETATM	65	H65	UNK	1	2.805	5.008	-2.613	1.00	0.00	H
HETATM	66	H66	UNK	1	1.454	3.906	-2.375	1.00	0.00	H
HETATM	67	H67	UNK	1	1.905	-0.516	-3.940	1.00	0.00	H
HETATM	68	H68	UNK	1	3.297	-0.803	-4.971	1.00	0.00	H
HETATM	69	H69	UNK	1	0.324	-4.527	-1.997	1.00	0.00	H
HETATM	70	H70	UNK	1	1.447	-5.840	-1.678	1.00	0.00	H
HETATM	71	H71	UNK	1	5.589	0.113	-4.061	1.00	0.00	H
HETATM	72	H72	UNK	1	5.354	-1.974	-3.587	1.00	0.00	H
HETATM	73	H73	UNK	1	2.667	5.087	3.212	1.00	0.00	H
HETATM	74	H74	UNK	1	-2.264	-0.997	6.760	1.00	0.00	H
HETATM	75	H75	UNK	1	5.138	4.129	-2.657	1.00	0.00	H
HETATM	76	H76	UNK	1	0.437	-3.790	-4.126	1.00	0.00	H
HETATM	77	H77	UNK	1	0.913	-2.264	-4.878	1.00	0.00	H
HETATM	78	C78	UNK	1	-2.966	3.717	3.676	1.00	0.00	C
HETATM	79	C79	UNK	1	-4.116	-1.059	2.023	1.00	0.00	C
HETATM	80	C80	UNK	1	-0.509	5.276	-0.756	1.00	0.00	C
HETATM	81	C81	UNK	1	0.774	1.924	-4.097	1.00	0.00	C
HETATM	82	C82	UNK	1	-2.050	-5.581	-0.668	1.00	0.00	C
HETATM	83	H83	UNK	1	0.009	5.721	-1.617	1.00	0.00	H
HETATM	84	H84	UNK	1	-3.227	3.256	4.638	1.00	0.00	H
HETATM	85	H85	UNK	1	-4.541	-0.626	2.933	1.00	0.00	H
HETATM	86	H86	UNK	1	-0.416	5.980	0.081	1.00	0.00	H
HETATM	87	H87	UNK	1	1.186	2.891	-4.410	1.00	0.00	H
HETATM	88	H88	UNK	1	1.020	1.198	-4.882	1.00	0.00	H
HETATM	89	H89	UNK	1	-1.324	-6.314	-1.044	1.00	0.00	H
HETATM	90	H90	UNK	1	-2.353	4.604	3.890	1.00	0.00	H
HETATM	91	C109	UNK	1	6.169	-4.484	-2.682	1.00	0.00	C
HETATM	92	C110	UNK	1	6.646	-4.887	-1.268	1.00	0.00	C
HETATM	93	H111	UNK	1	6.779	-4.009	-0.628	1.00	0.00	H
HETATM	94	H112	UNK	1	5.941	-5.560	-0.771	1.00	0.00	H
HETATM	95	H113	UNK	1	7.609	-5.406	-1.325	1.00	0.00	H
HETATM	96	C114	UNK	1	6.048	-5.758	-3.555	1.00	0.00	C
HETATM	97	H115	UNK	1	5.339	-6.476	-3.132	1.00	0.00	H
HETATM	98	H116	UNK	1	5.711	-5.509	-4.566	1.00	0.00	H
HETATM	99	H117	UNK	1	7.020	-6.258	-3.634	1.00	0.00	H
HETATM	100	C118	UNK	1	7.241	-3.576	-3.314	1.00	0.00	C
HETATM	101	H119	UNK	1	8.203	-4.098	-3.330	1.00	0.00	H
HETATM	102	H120	UNK	1	6.995	-3.312	-4.347	1.00	0.00	H
HETATM	103	H121	UNK	1	7.378	-2.649	-2.748	1.00	0.00	H
HETATM	104	C122	UNK	1	-1.934	-3.616	7.492	1.00	0.00	C
HETATM	105	C123	UNK	1	-1.730	-5.143	7.481	1.00	0.00	C
HETATM	106	H124	UNK	1	-2.570	-5.664	7.010	1.00	0.00	H
HETATM	107	H125	UNK	1	-0.811	-5.430	6.959	1.00	0.00	H
HETATM	108	H126	UNK	1	-1.651	-5.511	8.508	1.00	0.00	H
HETATM	109	C127	UNK	1	-0.725	-2.974	8.212	1.00	0.00	C
HETATM	110	H128	UNK	1	0.207	-3.180	7.674	1.00	0.00	H
HETATM	111	H129	UNK	1	-0.829	-1.889	8.301	1.00	0.00	H
HETATM	112	H130	UNK	1	-0.626	-3.380	9.225	1.00	0.00	H
HETATM	113	C131	UNK	1	-3.225	-3.307	8.287	1.00	0.00	C
HETATM	114	H132	UNK	1	-3.151	-3.708	9.304	1.00	0.00	H
HETATM	115	H133	UNK	1	-3.407	-2.231	8.366	1.00	0.00	H
HETATM	116	H134	UNK	1	-4.099	-3.760	7.807	1.00	0.00	H
HETATM	117	C135	UNK	1	2.969	-4.982	3.313	1.00	0.00	C

HETATM	118	C136	UNK	1	2.548	-4.822	4.786	1.00	0.00	C
HETATM	119	H137	UNK	1	2.189	-3.810	5.001	1.00	0.00	H
HETATM	120	H138	UNK	1	1.763	-5.531	5.067	1.00	0.00	H
HETATM	121	H139	UNK	1	3.407	-5.012	5.436	1.00	0.00	H
HETATM	122	C140	UNK	1	4.138	-4.010	3.039	1.00	0.00	C
HETATM	123	H141	UNK	1	3.830	-2.968	3.170	1.00	0.00	H
HETATM	124	H142	UNK	1	4.963	-4.207	3.733	1.00	0.00	H
HETATM	125	H143	UNK	1	4.533	-4.117	2.025	1.00	0.00	H
HETATM	126	C144	UNK	1	3.461	-6.436	3.109	1.00	0.00	C
HETATM	127	H145	UNK	1	4.288	-6.658	3.791	1.00	0.00	H
HETATM	128	H146	UNK	1	2.657	-7.153	3.304	1.00	0.00	H
HETATM	129	H147	UNK	1	3.817	-6.603	2.087	1.00	0.00	H
HETATM	130	C148	UNK	1	2.556	0.751	5.361	1.00	0.00	C
HETATM	131	C149	UNK	1	2.310	-0.511	6.209	1.00	0.00	C
HETATM	132	H150	UNK	1	1.942	-1.344	5.601	1.00	0.00	H
HETATM	133	H151	UNK	1	3.247	-0.829	6.675	1.00	0.00	H
HETATM	134	H152	UNK	1	1.588	-0.330	7.012	1.00	0.00	H
HETATM	135	C153	UNK	1	3.085	1.862	6.299	1.00	0.00	C
HETATM	136	H154	UNK	1	2.342	2.119	7.061	1.00	0.00	H
HETATM	137	H155	UNK	1	3.995	1.529	6.810	1.00	0.00	H
HETATM	138	H156	UNK	1	3.329	2.776	5.749	1.00	0.00	H
HETATM	139	C157	UNK	1	3.637	0.419	4.308	1.00	0.00	C
HETATM	140	H158	UNK	1	4.560	0.094	4.800	1.00	0.00	H
HETATM	141	H159	UNK	1	3.308	-0.388	3.644	1.00	0.00	H
HETATM	142	H160	UNK	1	3.881	1.281	3.681	1.00	0.00	H
HETATM	143	C161	UNK	1	5.099	5.557	2.060	1.00	0.00	C
HETATM	144	C162	UNK	1	6.290	5.621	1.085	1.00	0.00	C
HETATM	145	H163	UNK	1	6.093	6.293	0.243	1.00	0.00	H
HETATM	146	H164	UNK	1	7.172	6.005	1.607	1.00	0.00	H
HETATM	147	H165	UNK	1	6.551	4.636	0.683	1.00	0.00	H
HETATM	148	C166	UNK	1	4.836	6.986	2.591	1.00	0.00	C
HETATM	149	H167	UNK	1	4.570	7.665	1.775	1.00	0.00	H
HETATM	150	H168	UNK	1	4.020	7.003	3.321	1.00	0.00	H
HETATM	151	H169	UNK	1	5.731	7.381	3.083	1.00	0.00	H
HETATM	152	C170	UNK	1	5.493	4.642	3.243	1.00	0.00	C
HETATM	153	H171	UNK	1	6.415	5.002	3.712	1.00	0.00	H
HETATM	154	H172	UNK	1	4.720	4.617	4.017	1.00	0.00	H
HETATM	155	H173	UNK	1	5.662	3.613	2.908	1.00	0.00	H
HETATM	156	C174	UNK	1	7.035	2.464	-3.689	1.00	0.00	C
HETATM	157	C175	UNK	1	7.069	3.492	-4.845	1.00	0.00	C
HETATM	158	H176	UNK	1	6.577	3.096	-5.740	1.00	0.00	H
HETATM	159	H177	UNK	1	6.565	4.425	-4.573	1.00	0.00	H
HETATM	160	H178	UNK	1	8.104	3.736	-5.107	1.00	0.00	H
HETATM	161	C179	UNK	1	7.744	3.064	-2.454	1.00	0.00	C
HETATM	162	H180	UNK	1	7.268	3.990	-2.116	1.00	0.00	H
HETATM	163	H181	UNK	1	7.749	2.359	-1.618	1.00	0.00	H
HETATM	164	H182	UNK	1	8.784	3.304	-2.699	1.00	0.00	H
HETATM	165	C183	UNK	1	7.823	1.215	-4.130	1.00	0.00	C
HETATM	166	H184	UNK	1	8.863	1.490	-4.327	1.00	0.00	H
HETATM	167	H185	UNK	1	7.827	0.445	-3.352	1.00	0.00	H
HETATM	168	H186	UNK	1	7.423	0.779	-5.051	1.00	0.00	H
HETATM	169	C187	UNK	1	-1.138	-2.314	-4.198	1.00	0.00	C
HETATM	170	H188	UNK	1	-1.708	-2.768	-3.381	1.00	0.00	H
HETATM	171	H189	UNK	1	-1.245	-1.228	-4.094	1.00	0.00	H
HETATM	172	C190	UNK	1	-1.699	-2.770	-5.554	1.00	0.00	C
HETATM	173	H191	UNK	1	-1.114	-2.311	-6.363	1.00	0.00	H
HETATM	174	H192	UNK	1	-1.560	-3.855	-5.659	1.00	0.00	H
HETATM	175	C193	UNK	1	-3.181	-2.433	-5.753	1.00	0.00	C
HETATM	176	H194	UNK	1	-3.770	-2.904	-4.953	1.00	0.00	H
HETATM	177	H195	UNK	1	-3.325	-1.348	-5.643	1.00	0.00	H
HETATM	178	C196	UNK	1	-3.729	-2.880	-7.114	1.00	0.00	C
HETATM	179	H197	UNK	1	-3.140	-2.410	-7.913	1.00	0.00	H

HETATM	180	H198	UNK	1	-3.581	-3.962	-7.225	1.00	0.00	H
HETATM	181	C199	UNK	1	-5.211	-2.545	-7.308	1.00	0.00	C
HETATM	182	H200	UNK	1	-5.831	-3.034	-6.548	1.00	0.00	H
HETATM	183	H201	UNK	1	-5.385	-1.465	-7.238	1.00	0.00	H
HETATM	184	H202	UNK	1	-5.569	-2.874	-8.288	1.00	0.00	H
HETATM	185	C203	UNK	1	-0.728	2.031	-3.912	1.00	0.00	C
HETATM	186	H204	UNK	1	-1.133	1.068	-3.580	1.00	0.00	H
HETATM	187	H205	UNK	1	-0.937	2.748	-3.111	1.00	0.00	H
HETATM	188	C206	UNK	1	-1.408	2.470	-5.219	1.00	0.00	C
HETATM	189	H207	UNK	1	-0.947	3.403	-5.572	1.00	0.00	H
HETATM	190	H208	UNK	1	-1.209	1.723	-6.000	1.00	0.00	H
HETATM	191	C209	UNK	1	-2.922	2.678	-5.097	1.00	0.00	C
HETATM	192	H210	UNK	1	-3.393	1.756	-4.732	1.00	0.00	H
HETATM	193	H211	UNK	1	-3.122	3.441	-4.332	1.00	0.00	H
HETATM	194	C212	UNK	1	-3.583	3.101	-6.415	1.00	0.00	C
HETATM	195	H213	UNK	1	-3.099	4.016	-6.785	1.00	0.00	H
HETATM	196	H214	UNK	1	-3.395	2.332	-7.176	1.00	0.00	H
HETATM	197	C215	UNK	1	-5.091	3.336	-6.287	1.00	0.00	C
HETATM	198	H216	UNK	1	-5.608	2.432	-5.948	1.00	0.00	H
HETATM	199	H217	UNK	1	-5.307	4.129	-5.562	1.00	0.00	H
HETATM	200	H218	UNK	1	-5.529	3.635	-7.244	1.00	0.00	H
HETATM	201	C219	UNK	1	-4.946	-2.257	1.569	1.00	0.00	C
HETATM	202	H220	UNK	1	-4.467	-2.693	0.684	1.00	0.00	H
HETATM	203	H221	UNK	1	-4.938	-3.025	2.352	1.00	0.00	H
HETATM	204	C222	UNK	1	-6.400	-1.889	1.221	1.00	0.00	C
HETATM	205	H223	UNK	1	-6.402	-1.110	0.446	1.00	0.00	H
HETATM	206	H224	UNK	1	-6.874	-2.766	0.764	1.00	0.00	H
HETATM	207	C225	UNK	1	-7.259	-1.431	2.409	1.00	0.00	C
HETATM	208	H226	UNK	1	-7.214	-2.190	3.203	1.00	0.00	H
HETATM	209	H227	UNK	1	-6.846	-0.511	2.846	1.00	0.00	H
HETATM	210	C228	UNK	1	-8.725	-1.183	2.030	1.00	0.00	C
HETATM	211	H229	UNK	1	-8.768	-0.434	1.227	1.00	0.00	H
HETATM	212	H230	UNK	1	-9.147	-2.104	1.605	1.00	0.00	H
HETATM	213	C231	UNK	1	-9.585	-0.721	3.209	1.00	0.00	C
HETATM	214	H232	UNK	1	-9.589	-1.465	4.013	1.00	0.00	H
HETATM	215	H233	UNK	1	-9.210	0.218	3.631	1.00	0.00	H
HETATM	216	H234	UNK	1	-10.624	-0.556	2.905	1.00	0.00	H
HETATM	217	C235	UNK	1	-3.145	-5.329	-1.693	1.00	0.00	C
HETATM	218	H236	UNK	1	-3.821	-4.557	-1.303	1.00	0.00	H
HETATM	219	H237	UNK	1	-2.689	-4.920	-2.604	1.00	0.00	H
HETATM	220	C238	UNK	1	-3.943	-6.594	-2.035	1.00	0.00	C
HETATM	221	H239	UNK	1	-3.259	-7.373	-2.397	1.00	0.00	H
HETATM	222	H240	UNK	1	-4.404	-6.994	-1.121	1.00	0.00	H
HETATM	223	C241	UNK	1	-5.033	-6.349	-3.086	1.00	0.00	C
HETATM	224	H242	UNK	1	-5.714	-5.564	-2.727	1.00	0.00	H
HETATM	225	H243	UNK	1	-4.570	-5.954	-4.002	1.00	0.00	H
HETATM	226	C244	UNK	1	-5.845	-7.603	-3.431	1.00	0.00	C
HETATM	227	H245	UNK	1	-5.165	-8.389	-3.785	1.00	0.00	H
HETATM	228	H246	UNK	1	-6.311	-7.994	-2.517	1.00	0.00	H
HETATM	229	C247	UNK	1	-6.925	-7.348	-4.487	1.00	0.00	C
HETATM	230	H248	UNK	1	-7.642	-6.592	-4.147	1.00	0.00	H
HETATM	231	H249	UNK	1	-6.487	-6.990	-5.425	1.00	0.00	H
HETATM	232	H250	UNK	1	-7.487	-8.260	-4.710	1.00	0.00	H
HETATM	233	C251	UNK	1	-1.975	5.031	-1.075	1.00	0.00	C
HETATM	234	H252	UNK	1	-2.055	4.312	-1.899	1.00	0.00	H
HETATM	235	H253	UNK	1	-2.454	4.570	-0.202	1.00	0.00	H
HETATM	236	C254	UNK	1	-2.709	6.328	-1.446	1.00	0.00	C
HETATM	237	H255	UNK	1	-2.608	7.052	-0.625	1.00	0.00	H
HETATM	238	H256	UNK	1	-2.224	6.788	-2.318	1.00	0.00	H
HETATM	239	C257	UNK	1	-4.197	6.114	-1.748	1.00	0.00	C
HETATM	240	H258	UNK	1	-4.302	5.395	-2.574	1.00	0.00	H
HETATM	241	H259	UNK	1	-4.681	5.650	-0.876	1.00	0.00	H

HETATM	242	C260	UNK	1	-4.941	7.407	-2.109	1.00	0.00	C
HETATM	243	H261	UNK	1	-4.831	8.127	-1.287	1.00	0.00	H
HETATM	244	H262	UNK	1	-4.460	7.868	-2.982	1.00	0.00	H
HETATM	245	C263	UNK	1	-6.428	7.186	-2.400	1.00	0.00	C
HETATM	246	H264	UNK	1	-6.570	6.495	-3.239	1.00	0.00	H
HETATM	247	H265	UNK	1	-6.944	6.762	-1.531	1.00	0.00	H
HETATM	248	H266	UNK	1	-6.927	8.125	-2.656	1.00	0.00	H
HETATM	249	C267	UNK	1	-4.220	4.099	2.904	1.00	0.00	C
HETATM	250	H268	UNK	1	-3.921	4.522	1.936	1.00	0.00	H
HETATM	251	H269	UNK	1	-4.788	3.187	2.684	1.00	0.00	H
HETATM	252	C270	UNK	1	-5.104	5.100	3.659	1.00	0.00	C
HETATM	253	H271	UNK	1	-5.388	4.678	4.633	1.00	0.00	H
HETATM	254	H272	UNK	1	-4.526	6.009	3.879	1.00	0.00	H
HETATM	255	C273	UNK	1	-6.372	5.483	2.885	1.00	0.00	C
HETATM	256	H274	UNK	1	-6.088	5.899	1.907	1.00	0.00	H
HETATM	257	H275	UNK	1	-6.953	4.575	2.671	1.00	0.00	H
HETATM	258	C276	UNK	1	-7.261	6.491	3.623	1.00	0.00	C
HETATM	259	H277	UNK	1	-7.542	6.077	4.601	1.00	0.00	H
HETATM	260	H278	UNK	1	-6.681	7.399	3.833	1.00	0.00	H
HETATM	261	C279	UNK	1	-8.526	6.861	2.843	1.00	0.00	C
HETATM	262	H280	UNK	1	-8.278	7.309	1.873	1.00	0.00	H
HETATM	263	H281	UNK	1	-9.146	5.978	2.650	1.00	0.00	H
HETATM	264	H282	UNK	1	-9.138	7.582	3.393	1.00	0.00	H
HETATM	265	N91	UNK	1	0.570	-0.255	-0.465	1.00	0.00	N
HETATM	266	C92	UNK	1	-0.798	-0.134	0.202	1.00	0.00	C
HETATM	267	C93	UNK	1	-4.438	0.432	-2.063	1.00	0.00	C
HETATM	268	C94	UNK	1	-3.857	-0.843	-1.937	1.00	0.00	C
HETATM	269	C95	UNK	1	-2.655	-1.025	-1.258	1.00	0.00	C
HETATM	270	C96	UNK	1	-1.986	0.070	-0.694	1.00	0.00	C
HETATM	271	C97	UNK	1	-2.547	1.345	-0.827	1.00	0.00	C
HETATM	272	C98	UNK	1	-3.751	1.524	-1.503	1.00	0.00	C
HETATM	273	H99	UNK	1	-0.923	-1.048	0.784	1.00	0.00	H
HETATM	274	H100	UNK	1	-0.702	0.697	0.903	1.00	0.00	H
HETATM	275	H101	UNK	1	0.824	0.615	-0.957	1.00	0.00	H
HETATM	276	H102	UNK	1	0.557	-0.977	-1.207	1.00	0.00	H
HETATM	277	H103	UNK	1	-4.381	-1.708	-2.331	1.00	0.00	H
HETATM	278	H104	UNK	1	-2.262	-2.029	-1.117	1.00	0.00	H
HETATM	279	H105	UNK	1	-2.046	2.197	-0.378	1.00	0.00	H
HETATM	280	H106	UNK	1	-4.164	2.522	-1.601	1.00	0.00	H
HETATM	281	H107	UNK	1	1.401	-1.686	0.826	1.00	0.00	H
HETATM	282	H108	UNK	1	1.238	-0.066	1.510	1.00	0.00	H
HETATM	283	C283	UNK	1	-8.239	0.960	-4.013	1.00	0.00	C
HETATM	284	C284	UNK	1	-7.907	1.729	-2.896	1.00	0.00	C
HETATM	285	C285	UNK	1	-6.676	1.559	-2.267	1.00	0.00	C
HETATM	286	C286	UNK	1	-5.748	0.615	-2.739	1.00	0.00	C
HETATM	287	C287	UNK	1	-6.097	-0.155	-3.862	1.00	0.00	C
HETATM	288	C288	UNK	1	-7.328	0.016	-4.492	1.00	0.00	C
HETATM	289	H289	UNK	1	-9.198	1.092	-4.503	1.00	0.00	H
HETATM	290	H290	UNK	1	-8.613	2.458	-2.509	1.00	0.00	H
HETATM	291	H291	UNK	1	-6.441	2.146	-1.384	1.00	0.00	H
HETATM	292	H292	UNK	1	-5.390	-0.877	-4.259	1.00	0.00	H
HETATM	293	H293	UNK	1	-7.574	-0.585	-5.363	1.00	0.00	H
HETATM	294	C294	UNK	1	1.574	-0.626	0.634	1.00	0.00	C
HETATM	295	C295	UNK	1	5.827	0.117	0.405	1.00	0.00	C
HETATM	296	C296	UNK	1	4.913	1.183	0.474	1.00	0.00	C
HETATM	297	C297	UNK	1	3.541	0.955	0.487	1.00	0.00	C
HETATM	298	C298	UNK	1	3.033	-0.348	0.396	1.00	0.00	C
HETATM	299	C299	UNK	1	3.935	-1.411	0.286	1.00	0.00	C
HETATM	300	C300	UNK	1	5.308	-1.182	0.299	1.00	0.00	C
HETATM	301	H301	UNK	1	5.274	2.203	0.522	1.00	0.00	H
HETATM	302	H302	UNK	1	2.868	1.801	0.588	1.00	0.00	H
HETATM	303	H303	UNK	1	3.564	-2.428	0.230	1.00	0.00	H



HETATM	304	H304	UNK	1	5.984	-2.029	0.271	1.00	0.00	H
HETATM	305	C305	UNK	1	10.076	0.787	0.597	1.00	0.00	C
HETATM	306	C306	UNK	1	9.561	-0.235	-0.201	1.00	0.00	C
HETATM	307	C307	UNK	1	8.186	-0.451	-0.264	1.00	0.00	C
HETATM	308	C308	UNK	1	7.292	0.351	0.467	1.00	0.00	C
HETATM	309	C309	UNK	1	7.827	1.373	1.270	1.00	0.00	C
HETATM	310	C310	UNK	1	9.203	1.589	1.333	1.00	0.00	C
HETATM	311	H311	UNK	1	11.148	0.955	0.648	1.00	0.00	H
HETATM	312	H312	UNK	1	10.231	-0.863	-0.781	1.00	0.00	H
HETATM	313	H313	UNK	1	7.797	-1.237	-0.903	1.00	0.00	H
HETATM	314	H314	UNK	1	7.163	1.983	1.873	1.00	0.00	H
HETATM	315	H315	UNK	1	9.594	2.379	1.968	1.00	0.00	H
CONNECT	1	36	80							
CONNECT	2	8	78							
CONNECT	3	16	82							
CONNECT	4	6	79							
CONNECT	5	13	49							
CONNECT	6	4	11	32						
CONNECT	7	9	10	130						
CONNECT	8	2	23	28						
CONNECT	9	7	23	50						
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CONNECT 301 296
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CONNECT 306 305 307 312
CONNECT 307 306 308 313
CONNECT 308 295 307 309
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CONNECT 311 305
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CONNECT 315 310
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## Atomic coordinates of $2^+ \subset 1^{1,2,3-alt}$

HETATM	1	O1	UNK	1	2.652	-1.985	-3.479	1.00	0.00	O
HETATM	2	O2	UNK	1	-0.813	-4.930	-0.850	1.00	0.00	O
HETATM	3	O3	UNK	1	-2.769	0.633	2.449	1.00	0.00	O
HETATM	4	O4	UNK	1	-1.916	-2.720	2.278	1.00	0.00	O
HETATM	5	O5	UNK	1	0.583	2.781	0.627	1.00	0.00	O
HETATM	6	C6	UNK	1	-1.080	-3.042	3.343	1.00	0.00	C
HETATM	7	C7	UNK	1	3.196	-4.468	0.355	1.00	0.00	C
HETATM	8	C8	UNK	1	0.497	-4.706	-0.433	1.00	0.00	C
HETATM	9	C9	UNK	1	2.174	-4.635	1.295	1.00	0.00	C
HETATM	10	C10	UNK	1	2.812	-4.340	-0.987	1.00	0.00	C
HETATM	11	C11	UNK	1	-0.237	-4.166	3.230	1.00	0.00	C
HETATM	12	C12	UNK	1	-2.019	-1.050	4.650	1.00	0.00	C
HETATM	13	C13	UNK	1	-0.035	4.024	0.494	1.00	0.00	C
HETATM	14	C14	UNK	1	-1.447	2.501	3.243	1.00	0.00	C
HETATM	15	C15	UNK	1	-0.243	-5.049	1.988	1.00	0.00	C
HETATM	16	C16	UNK	1	-1.887	1.171	3.389	1.00	0.00	C
HETATM	17	C17	UNK	1	0.590	-4.476	4.312	1.00	0.00	C
HETATM	18	C18	UNK	1	-0.684	-0.857	-4.570	1.00	0.00	C
HETATM	19	C19	UNK	1	-1.465	0.364	4.461	1.00	0.00	C
HETATM	20	C20	UNK	1	0.523	-3.112	-3.436	1.00	0.00	C
HETATM	21	C21	UNK	1	-1.465	-1.997	-4.353	1.00	0.00	C
HETATM	22	C22	UNK	1	1.466	4.485	-1.528	1.00	0.00	C
HETATM	23	C23	UNK	1	0.827	-4.759	0.933	1.00	0.00	C
HETATM	24	C24	UNK	1	1.156	-4.390	-2.893	1.00	0.00	C
HETATM	25	C25	UNK	1	-0.206	2.287	5.344	1.00	0.00	C
HETATM	26	C26	UNK	1	-1.961	3.326	2.071	1.00	0.00	C
HETATM	27	C27	UNK	1	-0.619	0.947	5.410	1.00	0.00	C
HETATM	28	C28	UNK	1	1.483	-4.449	-1.404	1.00	0.00	C
HETATM	29	C29	UNK	1	-1.641	5.664	1.219	1.00	0.00	C
HETATM	30	C30	UNK	1	0.686	-0.810	-4.269	1.00	0.00	C
HETATM	31	C31	UNK	1	-0.146	6.182	-0.566	1.00	0.00	C
HETATM	32	C32	UNK	1	-1.068	-2.233	4.491	1.00	0.00	C
HETATM	33	C33	UNK	1	0.414	4.902	-0.509	1.00	0.00	C

HETATM	34	C34	UNK	1	-1.151	6.610	0.313	1.00	0.00	C
HETATM	35	C35	UNK	1	-1.127	4.361	1.316	1.00	0.00	C
HETATM	36	C36	UNK	1	1.287	-1.963	-3.729	1.00	0.00	C
HETATM	37	C37	UNK	1	-0.637	3.042	4.247	1.00	0.00	C
HETATM	38	C38	UNK	1	0.637	-3.700	5.482	1.00	0.00	C
HETATM	39	C39	UNK	1	-0.201	-2.584	5.538	1.00	0.00	C
HETATM	40	C40	UNK	1	-0.838	-3.098	-3.752	1.00	0.00	C
HETATM	41	C41	UNK	1	1.536	0.418	-4.613	1.00	0.00	C
HETATM	42	C42	UNK	1	-0.031	2.386	-4.993	1.00	0.00	C
HETATM	43	C43	UNK	1	-0.578	3.640	-4.675	1.00	0.00	C
HETATM	44	C44	UNK	1	-0.102	4.267	-3.520	1.00	0.00	C
HETATM	45	C45	UNK	1	0.925	3.723	-2.736	1.00	0.00	C
HETATM	46	C46	UNK	1	1.480	2.490	-3.123	1.00	0.00	C
HETATM	47	C47	UNK	1	0.969	1.778	-4.228	1.00	0.00	C
HETATM	48	O48	UNK	1	2.576	1.981	-2.436	1.00	0.00	O
HETATM	49	C49	UNK	1	1.560	2.699	1.718	1.00	0.00	C
HETATM	50	H50	UNK	1	2.422	-4.694	2.348	1.00	0.00	H
HETATM	51	H51	UNK	1	3.563	-4.179	-1.752	1.00	0.00	H
HETATM	52	H52	UNK	1	-2.437	-1.102	5.663	1.00	0.00	H
HETATM	53	H53	UNK	1	-2.844	-1.176	3.955	1.00	0.00	H
HETATM	54	H54	UNK	1	-1.214	-4.991	1.498	1.00	0.00	H
HETATM	55	H55	UNK	1	-0.121	-6.088	2.322	1.00	0.00	H
HETATM	56	H56	UNK	1	-3.825	-2.961	3.078	1.00	0.00	H
HETATM	57	H57	UNK	1	-1.137	0.023	-5.006	1.00	0.00	H
HETATM	58	H58	UNK	1	0.481	-5.213	-3.142	1.00	0.00	H
HETATM	59	H59	UNK	1	2.085	-4.581	-3.436	1.00	0.00	H
HETATM	60	H60	UNK	1	-4.350	1.663	1.590	1.00	0.00	H
HETATM	61	H61	UNK	1	-0.308	0.341	6.255	1.00	0.00	H
HETATM	62	H62	UNK	1	-2.471	5.921	1.867	1.00	0.00	H
HETATM	63	H63	UNK	1	-0.349	4.083	4.154	1.00	0.00	H
HETATM	64	H64	UNK	1	-0.222	-1.974	6.434	1.00	0.00	H
HETATM	65	H65	UNK	1	1.709	0.417	-5.698	1.00	0.00	H
HETATM	66	H66	UNK	1	2.505	0.291	-4.134	1.00	0.00	H
HETATM	67	H67	UNK	1	2.221	3.864	-1.053	1.00	0.00	H
HETATM	68	H68	UNK	1	1.970	5.392	-1.884	1.00	0.00	H
HETATM	69	H69	UNK	1	-2.316	2.626	1.311	1.00	0.00	H
HETATM	70	H70	UNK	1	-2.862	3.852	2.409	1.00	0.00	H
HETATM	71	H71	UNK	1	-0.512	5.223	-3.217	1.00	0.00	H
HETATM	72	H72	UNK	1	0.236	6.868	-1.318	1.00	0.00	H
HETATM	73	H73	UNK	1	-1.407	-3.998	-3.549	1.00	0.00	H
HETATM	74	H74	UNK	1	1.204	-5.369	4.242	1.00	0.00	H
HETATM	75	H75	UNK	1	-0.371	1.875	-5.889	1.00	0.00	H
HETATM	76	H76	UNK	1	1.600	1.638	1.952	1.00	0.00	H
HETATM	77	H77	UNK	1	1.148	3.219	2.583	1.00	0.00	H
HETATM	78	C78	UNK	1	-1.123	-6.330	-1.011	1.00	0.00	C
HETATM	79	C79	UNK	1	-3.190	-3.397	2.294	1.00	0.00	C
HETATM	80	C80	UNK	1	3.455	-2.316	-4.630	1.00	0.00	C
HETATM	81	C81	UNK	1	3.831	2.449	-2.977	1.00	0.00	C
HETATM	82	C82	UNK	1	-4.135	1.143	2.528	1.00	0.00	C
HETATM	83	H83	UNK	1	3.230	-1.624	-5.453	1.00	0.00	H
HETATM	84	H84	UNK	1	-0.390	-6.792	-1.687	1.00	0.00	H
HETATM	85	H85	UNK	1	-3.042	-4.454	2.546	1.00	0.00	H
HETATM	86	H86	UNK	1	3.201	-3.327	-4.978	1.00	0.00	H
HETATM	87	H87	UNK	1	3.877	2.209	-4.049	1.00	0.00	H
HETATM	88	H88	UNK	1	3.883	3.543	-2.885	1.00	0.00	H
HETATM	89	H89	UNK	1	-4.184	1.871	3.343	1.00	0.00	H
HETATM	90	H90	UNK	1	-1.036	-6.841	-0.042	1.00	0.00	H
HETATM	91	C109	UNK	1	-1.688	8.051	0.234	1.00	0.00	C
HETATM	92	C110	UNK	1	-2.772	8.331	1.291	1.00	0.00	C
HETATM	93	H111	UNK	1	-3.652	7.693	1.155	1.00	0.00	H
HETATM	94	H112	UNK	1	-2.397	8.184	2.309	1.00	0.00	H
HETATM	95	H113	UNK	1	-3.107	9.369	1.210	1.00	0.00	H

HETATM	96	C114	UNK	1	-0.522	9.043	0.467	1.00	0.00	C
HETATM	97	H115	UNK	1	-0.071	8.893	1.453	1.00	0.00	H
HETATM	98	H116	UNK	1	0.266	8.930	-0.282	1.00	0.00	H
HETATM	99	H117	UNK	1	-0.885	10.075	0.413	1.00	0.00	H
HETATM	100	C118	UNK	1	-2.300	8.303	-1.165	1.00	0.00	C
HETATM	101	H119	UNK	1	-2.672	9.331	-1.238	1.00	0.00	H
HETATM	102	H120	UNK	1	-1.567	8.159	-1.964	1.00	0.00	H
HETATM	103	H121	UNK	1	-3.141	7.627	-1.354	1.00	0.00	H
HETATM	104	C122	UNK	1	1.554	-4.119	6.647	1.00	0.00	C
HETATM	105	C123	UNK	1	1.503	-3.121	7.819	1.00	0.00	C
HETATM	106	H124	UNK	1	1.818	-2.117	7.514	1.00	0.00	H
HETATM	107	H125	UNK	1	0.500	-3.050	8.254	1.00	0.00	H
HETATM	108	H126	UNK	1	2.180	-3.451	8.613	1.00	0.00	H
HETATM	109	C127	UNK	1	1.109	-5.505	7.173	1.00	0.00	C
HETATM	110	H128	UNK	1	0.077	-5.472	7.539	1.00	0.00	H
HETATM	111	H129	UNK	1	1.163	-6.272	6.395	1.00	0.00	H
HETATM	112	H130	UNK	1	1.752	-5.823	8.000	1.00	0.00	H
HETATM	113	C131	UNK	1	3.018	-4.206	6.155	1.00	0.00	C
HETATM	114	H132	UNK	1	3.678	-4.502	6.977	1.00	0.00	H
HETATM	115	H133	UNK	1	3.138	-4.944	5.356	1.00	0.00	H
HETATM	116	H134	UNK	1	3.365	-3.241	5.773	1.00	0.00	H
HETATM	117	C135	UNK	1	0.663	2.878	6.472	1.00	0.00	C
HETATM	118	C136	UNK	1	-0.097	2.768	7.816	1.00	0.00	C
HETATM	119	H137	UNK	1	-1.041	3.321	7.779	1.00	0.00	H
HETATM	120	H138	UNK	1	-0.328	1.729	8.071	1.00	0.00	H
HETATM	121	H139	UNK	1	0.508	3.183	8.629	1.00	0.00	H
HETATM	122	C140	UNK	1	1.001	4.362	6.234	1.00	0.00	C
HETATM	123	H141	UNK	1	0.101	4.983	6.184	1.00	0.00	H
HETATM	124	H142	UNK	1	1.612	4.737	7.061	1.00	0.00	H
HETATM	125	H143	UNK	1	1.572	4.511	5.312	1.00	0.00	H
HETATM	126	C144	UNK	1	1.991	2.092	6.569	1.00	0.00	C
HETATM	127	H145	UNK	1	2.615	2.495	7.374	1.00	0.00	H
HETATM	128	H146	UNK	1	1.824	1.031	6.778	1.00	0.00	H
HETATM	129	H147	UNK	1	2.555	2.167	5.633	1.00	0.00	H
HETATM	130	C148	UNK	1	4.686	-4.537	0.745	1.00	0.00	C
HETATM	131	C149	UNK	1	5.186	-5.976	0.461	1.00	0.00	C
HETATM	132	H150	UNK	1	5.070	-6.234	-0.597	1.00	0.00	H
HETATM	133	H151	UNK	1	6.246	-6.073	0.720	1.00	0.00	H
HETATM	134	H152	UNK	1	4.624	-6.710	1.048	1.00	0.00	H
HETATM	135	C153	UNK	1	4.910	-4.228	2.239	1.00	0.00	C
HETATM	136	H154	UNK	1	4.453	-4.981	2.888	1.00	0.00	H
HETATM	137	H155	UNK	1	5.982	-4.226	2.460	1.00	0.00	H
HETATM	138	H156	UNK	1	4.507	-3.249	2.514	1.00	0.00	H
HETATM	139	C157	UNK	1	5.532	-3.547	-0.084	1.00	0.00	C
HETATM	140	H158	UNK	1	6.570	-3.563	0.264	1.00	0.00	H
HETATM	141	H159	UNK	1	5.547	-3.805	-1.146	1.00	0.00	H
HETATM	142	H160	UNK	1	5.150	-2.527	0.011	1.00	0.00	H
HETATM	143	C161	UNK	1	-2.930	-2.107	-4.821	1.00	0.00	C
HETATM	144	C162	UNK	1	-3.470	-0.780	-5.388	1.00	0.00	C
HETATM	145	H163	UNK	1	-2.910	-0.459	-6.272	1.00	0.00	H
HETATM	146	H164	UNK	1	-4.513	-0.908	-5.694	1.00	0.00	H
HETATM	147	H165	UNK	1	-3.438	0.026	-4.648	1.00	0.00	H
HETATM	148	C166	UNK	1	-3.009	-3.177	-5.938	1.00	0.00	C
HETATM	149	H167	UNK	1	-2.373	-2.906	-6.786	1.00	0.00	H
HETATM	150	H168	UNK	1	-2.687	-4.160	-5.580	1.00	0.00	H
HETATM	151	H169	UNK	1	-4.038	-3.273	-6.302	1.00	0.00	H
HETATM	152	C170	UNK	1	-3.843	-2.535	-3.650	1.00	0.00	C
HETATM	153	H171	UNK	1	-4.873	-2.666	-4.000	1.00	0.00	H
HETATM	154	H172	UNK	1	-3.523	-3.479	-3.201	1.00	0.00	H
HETATM	155	H173	UNK	1	-3.854	-1.773	-2.864	1.00	0.00	H
HETATM	156	C174	UNK	1	-1.636	4.273	-5.599	1.00	0.00	C
HETATM	157	C175	UNK	1	-1.034	4.455	-7.013	1.00	0.00	C



HETATM	158	H176	UNK	1	-0.157	5.110	-6.985	1.00	0.00	H
HETATM	159	H177	UNK	1	-0.725	3.502	-7.452	1.00	0.00	H
HETATM	160	H178	UNK	1	-1.772	4.905	-7.685	1.00	0.00	H
HETATM	161	C179	UNK	1	-2.875	3.351	-5.686	1.00	0.00	C
HETATM	162	H180	UNK	1	-2.623	2.367	-6.091	1.00	0.00	H
HETATM	163	H181	UNK	1	-3.325	3.204	-4.699	1.00	0.00	H
HETATM	164	H182	UNK	1	-3.633	3.794	-6.342	1.00	0.00	H
HETATM	165	C183	UNK	1	-2.099	5.655	-5.098	1.00	0.00	C
HETATM	166	H184	UNK	1	-2.841	6.066	-5.789	1.00	0.00	H
HETATM	167	H185	UNK	1	-2.568	5.598	-4.111	1.00	0.00	H
HETATM	168	H186	UNK	1	-1.270	6.367	-5.044	1.00	0.00	H
HETATM	169	C187	UNK	1	2.969	3.210	1.414	1.00	0.00	C
HETATM	170	H188	UNK	1	3.630	2.674	2.108	1.00	0.00	H
HETATM	171	H189	UNK	1	3.265	2.871	0.416	1.00	0.00	H
HETATM	172	C190	UNK	1	3.221	4.714	1.596	1.00	0.00	C
HETATM	173	H191	UNK	1	2.588	5.304	0.926	1.00	0.00	H
HETATM	174	H192	UNK	1	2.925	5.001	2.616	1.00	0.00	H
HETATM	175	C193	UNK	1	4.690	5.094	1.374	1.00	0.00	C
HETATM	176	H194	UNK	1	5.325	4.502	2.048	1.00	0.00	H
HETATM	177	H195	UNK	1	4.988	4.808	0.354	1.00	0.00	H
HETATM	178	C196	UNK	1	4.981	6.585	1.583	1.00	0.00	C
HETATM	179	H197	UNK	1	4.347	7.176	0.909	1.00	0.00	H
HETATM	180	H198	UNK	1	4.686	6.870	2.602	1.00	0.00	H
HETATM	181	C199	UNK	1	6.451	6.951	1.356	1.00	0.00	C
HETATM	182	H200	UNK	1	7.106	6.401	2.041	1.00	0.00	H
HETATM	183	H201	UNK	1	6.766	6.711	0.334	1.00	0.00	H
HETATM	184	H202	UNK	1	6.626	8.019	1.515	1.00	0.00	H
HETATM	185	C203	UNK	1	4.979	1.789	-2.231	1.00	0.00	C
HETATM	186	H204	UNK	1	4.896	2.031	-1.165	1.00	0.00	H
HETATM	187	H205	UNK	1	4.878	0.700	-2.320	1.00	0.00	H
HETATM	188	C206	UNK	1	6.352	2.234	-2.754	1.00	0.00	C
HETATM	189	H207	UNK	1	6.422	2.024	-3.831	1.00	0.00	H
HETATM	190	H208	UNK	1	6.447	3.324	-2.650	1.00	0.00	H
HETATM	191	C209	UNK	1	7.520	1.553	-2.030	1.00	0.00	C
HETATM	192	H210	UNK	1	7.439	1.743	-0.950	1.00	0.00	H
HETATM	193	H211	UNK	1	7.437	0.464	-2.154	1.00	0.00	H
HETATM	194	C212	UNK	1	8.897	2.014	-2.522	1.00	0.00	C
HETATM	195	H213	UNK	1	8.976	1.828	-3.602	1.00	0.00	H
HETATM	196	H214	UNK	1	8.981	3.102	-2.395	1.00	0.00	H
HETATM	197	C215	UNK	1	10.058	1.324	-1.799	1.00	0.00	C
HETATM	198	H216	UNK	1	10.025	1.520	-0.721	1.00	0.00	H
HETATM	199	H217	UNK	1	10.024	0.238	-1.940	1.00	0.00	H
HETATM	200	H218	UNK	1	11.025	1.676	-2.170	1.00	0.00	H
HETATM	201	C219	UNK	1	-3.838	-3.255	0.927	1.00	0.00	C
HETATM	202	H220	UNK	1	-3.923	-2.185	0.696	1.00	0.00	H
HETATM	203	H221	UNK	1	-3.171	-3.690	0.173	1.00	0.00	H
HETATM	204	C222	UNK	1	-5.224	-3.913	0.865	1.00	0.00	C
HETATM	205	H223	UNK	1	-5.127	-4.988	1.071	1.00	0.00	H
HETATM	206	H224	UNK	1	-5.859	-3.509	1.665	1.00	0.00	H
HETATM	207	C225	UNK	1	-5.928	-3.719	-0.483	1.00	0.00	C
HETATM	208	H226	UNK	1	-6.037	-2.643	-0.683	1.00	0.00	H
HETATM	209	H227	UNK	1	-5.292	-4.112	-1.287	1.00	0.00	H
HETATM	210	C228	UNK	1	-7.308	-4.385	-0.558	1.00	0.00	C
HETATM	211	H229	UNK	1	-7.199	-5.462	-0.368	1.00	0.00	H
HETATM	212	H230	UNK	1	-7.941	-3.998	0.252	1.00	0.00	H
HETATM	213	C231	UNK	1	-8.008	-4.172	-1.903	1.00	0.00	C
HETATM	214	H232	UNK	1	-8.165	-3.106	-2.104	1.00	0.00	H
HETATM	215	H233	UNK	1	-7.414	-4.580	-2.728	1.00	0.00	H
HETATM	216	H234	UNK	1	-8.987	-4.660	-1.926	1.00	0.00	H
HETATM	217	C235	UNK	1	-5.147	0.028	2.753	1.00	0.00	C
HETATM	218	H236	UNK	1	-5.045	-0.716	1.955	1.00	0.00	H
HETATM	219	H237	UNK	1	-4.930	-0.484	3.697	1.00	0.00	H

HETATM	220	C238	UNK	1	-6.586	0.564	2.779	1.00	0.00	C
HETATM	221	H239	UNK	1	-6.684	1.308	3.583	1.00	0.00	H
HETATM	222	H240	UNK	1	-6.795	1.101	1.843	1.00	0.00	H
HETATM	223	C241	UNK	1	-7.635	-0.537	2.979	1.00	0.00	C
HETATM	224	H242	UNK	1	-7.543	-1.277	2.171	1.00	0.00	H
HETATM	225	H243	UNK	1	-7.421	-1.078	3.912	1.00	0.00	H
HETATM	226	C244	UNK	1	-9.075	-0.011	3.020	1.00	0.00	C
HETATM	227	H245	UNK	1	-9.169	0.723	3.831	1.00	0.00	H
HETATM	228	H246	UNK	1	-9.287	0.536	2.091	1.00	0.00	H
HETATM	229	C247	UNK	1	-10.115	-1.119	3.210	1.00	0.00	C
HETATM	230	H248	UNK	1	-10.071	-1.850	2.394	1.00	0.00	H
HETATM	231	H249	UNK	1	-9.951	-1.660	4.148	1.00	0.00	H
HETATM	232	H250	UNK	1	-11.131	-0.712	3.236	1.00	0.00	H
HETATM	233	C251	UNK	1	4.923	-2.229	-4.245	1.00	0.00	C
HETATM	234	H252	UNK	1	5.135	-1.213	-3.886	1.00	0.00	H
HETATM	235	H253	UNK	1	5.109	-2.901	-3.398	1.00	0.00	H
HETATM	236	C254	UNK	1	5.860	-2.579	-5.408	1.00	0.00	C
HETATM	237	H255	UNK	1	5.636	-3.593	-5.766	1.00	0.00	H
HETATM	238	H256	UNK	1	5.660	-1.907	-6.255	1.00	0.00	H
HETATM	239	C257	UNK	1	7.345	-2.492	-5.034	1.00	0.00	C
HETATM	240	H258	UNK	1	7.569	-1.478	-4.673	1.00	0.00	H
HETATM	241	H259	UNK	1	7.547	-3.166	-4.190	1.00	0.00	H
HETATM	242	C260	UNK	1	8.289	-2.836	-6.193	1.00	0.00	C
HETATM	243	H261	UNK	1	8.063	-3.848	-6.554	1.00	0.00	H
HETATM	244	H262	UNK	1	8.086	-2.161	-7.036	1.00	0.00	H
HETATM	245	C263	UNK	1	9.769	-2.747	-5.812	1.00	0.00	C
HETATM	246	H264	UNK	1	10.033	-1.737	-5.478	1.00	0.00	H
HETATM	247	H265	UNK	1	10.011	-3.438	-4.996	1.00	0.00	H
HETATM	248	H266	UNK	1	10.415	-2.995	-6.660	1.00	0.00	H
HETATM	249	C267	UNK	1	-2.531	-6.473	-1.566	1.00	0.00	C
HETATM	250	H268	UNK	1	-3.234	-5.972	-0.889	1.00	0.00	H
HETATM	251	H269	UNK	1	-2.591	-5.947	-2.528	1.00	0.00	H
HETATM	252	C270	UNK	1	-2.942	-7.940	-1.751	1.00	0.00	C
HETATM	253	H271	UNK	1	-2.219	-8.443	-2.408	1.00	0.00	H
HETATM	254	H272	UNK	1	-2.887	-8.459	-0.784	1.00	0.00	H
HETATM	255	C273	UNK	1	-4.351	-8.104	-2.334	1.00	0.00	C
HETATM	256	H274	UNK	1	-5.076	-7.596	-1.682	1.00	0.00	H
HETATM	257	H275	UNK	1	-4.404	-7.589	-3.305	1.00	0.00	H
HETATM	258	C276	UNK	1	-4.772	-9.567	-2.515	1.00	0.00	C
HETATM	259	H277	UNK	1	-4.044	-10.075	-3.162	1.00	0.00	H
HETATM	260	H278	UNK	1	-4.723	-10.079	-1.544	1.00	0.00	H
HETATM	261	C279	UNK	1	-6.176	-9.723	-3.105	1.00	0.00	C
HETATM	262	H280	UNK	1	-6.931	-9.254	-2.464	1.00	0.00	H
HETATM	263	H281	UNK	1	-6.245	-9.255	-4.093	1.00	0.00	H
HETATM	264	H282	UNK	1	-6.446	-10.778	-3.219	1.00	0.00	H
HETATM	265	N91	UNK	1	-0.801	0.132	0.116	1.00	0.00	N
HETATM	266	C92	UNK	1	0.168	-1.060	0.176	1.00	0.00	C
HETATM	267	C93	UNK	1	3.918	-0.309	2.233	1.00	0.00	C
HETATM	268	C94	UNK	1	2.770	-0.703	2.943	1.00	0.00	C
HETATM	269	C95	UNK	1	1.563	-0.935	2.289	1.00	0.00	C
HETATM	270	C96	UNK	1	1.457	-0.781	0.901	1.00	0.00	C
HETATM	271	C97	UNK	1	2.598	-0.403	0.180	1.00	0.00	C
HETATM	272	C98	UNK	1	3.803	-0.169	0.838	1.00	0.00	C
HETATM	273	H99	UNK	1	-0.402	-1.871	0.633	1.00	0.00	H
HETATM	274	H100	UNK	1	0.374	-1.321	-0.863	1.00	0.00	H
HETATM	275	H101	UNK	1	-0.284	1.031	0.174	1.00	0.00	H
HETATM	276	H102	UNK	1	-1.444	0.118	0.926	1.00	0.00	H
HETATM	277	H103	UNK	1	2.824	-0.856	4.016	1.00	0.00	H
HETATM	278	H104	UNK	1	0.704	-1.249	2.868	1.00	0.00	H
HETATM	279	H105	UNK	1	2.550	-0.280	-0.898	1.00	0.00	H
HETATM	280	H106	UNK	1	4.663	0.151	0.261	1.00	0.00	H
HETATM	281	H107	UNK	1	-1.980	-0.955	-1.237	1.00	0.00	H

HETATM	282	H108	UNK	1	-0.917	0.243	-1.976	1.00	0.00	H
HETATM	283	C283	UNK	1	7.637	0.494	4.249	1.00	0.00	C
HETATM	284	C284	UNK	1	7.638	-0.053	2.965	1.00	0.00	C
HETATM	285	C285	UNK	1	6.435	-0.316	2.312	1.00	0.00	C
HETATM	286	C286	UNK	1	5.202	-0.040	2.929	1.00	0.00	C
HETATM	287	C287	UNK	1	5.219	0.509	4.223	1.00	0.00	C
HETATM	288	C288	UNK	1	6.422	0.772	4.875	1.00	0.00	C
HETATM	289	H289	UNK	1	8.575	0.699	4.757	1.00	0.00	H
HETATM	290	H290	UNK	1	8.578	-0.283	2.472	1.00	0.00	H
HETATM	291	H291	UNK	1	6.454	-0.766	1.324	1.00	0.00	H
HETATM	292	H292	UNK	1	4.282	0.750	4.716	1.00	0.00	H
HETATM	293	H293	UNK	1	6.410	1.203	5.872	1.00	0.00	H
HETATM	294	C294	UNK	1	-1.625	0.075	-1.163	1.00	0.00	C
HETATM	295	C295	UNK	1	-4.948	2.860	-1.392	1.00	0.00	C
HETATM	296	C296	UNK	1	-3.621	3.296	-1.557	1.00	0.00	C
HETATM	297	C297	UNK	1	-2.554	2.405	-1.483	1.00	0.00	C
HETATM	298	C298	UNK	1	-2.772	1.048	-1.214	1.00	0.00	C
HETATM	299	C299	UNK	1	-4.092	0.604	-1.056	1.00	0.00	C
HETATM	300	C300	UNK	1	-5.162	1.492	-1.150	1.00	0.00	C
HETATM	301	H301	UNK	1	-3.423	4.340	-1.775	1.00	0.00	H
HETATM	302	H302	UNK	1	-1.547	2.771	-1.657	1.00	0.00	H
HETATM	303	H303	UNK	1	-4.287	-0.447	-0.861	1.00	0.00	H
HETATM	304	H304	UNK	1	-6.174	1.124	-1.013	1.00	0.00	H
HETATM	305	C305	UNK	1	-8.232	5.625	-1.626	1.00	0.00	C
HETATM	306	C306	UNK	1	-7.032	6.008	-1.024	1.00	0.00	C
HETATM	307	C307	UNK	1	-5.967	5.111	-0.950	1.00	0.00	C
HETATM	308	C308	UNK	1	-6.082	3.813	-1.476	1.00	0.00	C
HETATM	309	C309	UNK	1	-7.296	3.442	-2.078	1.00	0.00	C
HETATM	310	C310	UNK	1	-8.359	4.339	-2.154	1.00	0.00	C
HETATM	311	H311	UNK	1	-9.061	6.324	-1.684	1.00	0.00	H
HETATM	312	H312	UNK	1	-6.927	7.004	-0.604	1.00	0.00	H
HETATM	313	H313	UNK	1	-5.047	5.408	-0.456	1.00	0.00	H
HETATM	314	H314	UNK	1	-7.397	2.453	-2.517	1.00	0.00	H
HETATM	315	H315	UNK	1	-9.286	4.037	-2.632	1.00	0.00	H
CONNECT	1	36	80							
CONNECT	2	8	78							
CONNECT	3	16	82							
CONNECT	4	6	79							
CONNECT	5	13	49							
CONNECT	6	4	11	32						
CONNECT	7	9	10	130						
CONNECT	8	2	23	28						
CONNECT	9	7	23	50						
CONNECT	10	7	28	51						
CONNECT	11	6	15	17						
CONNECT	12	19	32	52	53					
CONNECT	13	5	33	35						
CONNECT	14	16	26	37						
CONNECT	15	11	23	54	55					
CONNECT	16	3	14	19						
CONNECT	17	11	38	74						
CONNECT	18	21	30	57						
CONNECT	19	12	16	27						
CONNECT	20	24	36	40						
CONNECT	21	18	40	143						
CONNECT	22	33	45	67	68					
CONNECT	23	8	9	15						
CONNECT	24	20	28	58	59					
CONNECT	25	27	37	117						
CONNECT	26	14	35	69	70					
CONNECT	27	19	25	61						
CONNECT	28	8	10	24						

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