

Influence of Hydrophobic Residue on the Binding of CB[7] Toward Diammonium Ions of Common Ammonium•••Ammonium Distance

Supporting Information

Liping Cao,^a Āani Škalamera,^b Peter Y. Zavalij,^a Jiří Hostaš,^c Pavel Hobza,^{c,d,}
Kata Mlinarić-Majerski,^{b,*} Robert Glaser,^{e,*} Lyle Isaacs^{a,*}*

^aDepartment of Chemistry and Biochemistry, University of Maryland, College Park, Maryland
20742, United States;

^bDepartment of Organic Chemistry and Biochemistry, Ruđer Bošković Institute,
Bijenička cesta 54, 10000 Zagreb, Croatia;

^cInstitute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic,
16610 Praha 6, Czech Republic

^dRegional Center of Advanced Technologies and Materials, Department of Physical Chemistry,
Palacký University, 771 46 Olomouc, Czech Republic

^eDepartment of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

Table of Contents	Pages
¹ H and ¹³ C NMR spectra for 14	S2 – S3
¹ H NMR spectra recorded for selected CB[7]•guest complexes.	S4 – S11
Determination of K_{rel} for the competition between 14 and 5 for CB[7]	S12
Determination of K_a for CB[7]• 14 by competition of 14 and 5 for a limiting quantity of CB[7].....	S12 – S13
Selected ¹ H NMR spectra from the K_a and K_{rel} measurements.....	S13 – S21
Illustration of solvating H ₂ O molecules in the structure of CB[7]• 14	S23
Coordinates of the minimized geometry of CB[7] complexes of Guests 1b , 3b , 3c , 9 , and 14	S24-S44
Plot of ΔG_{exptl} versus ΔG_{calcd}	S45
C-H•••O close contacts in CB[7]• 3b , CB[7]• 9 and CB[7]• 14	S46

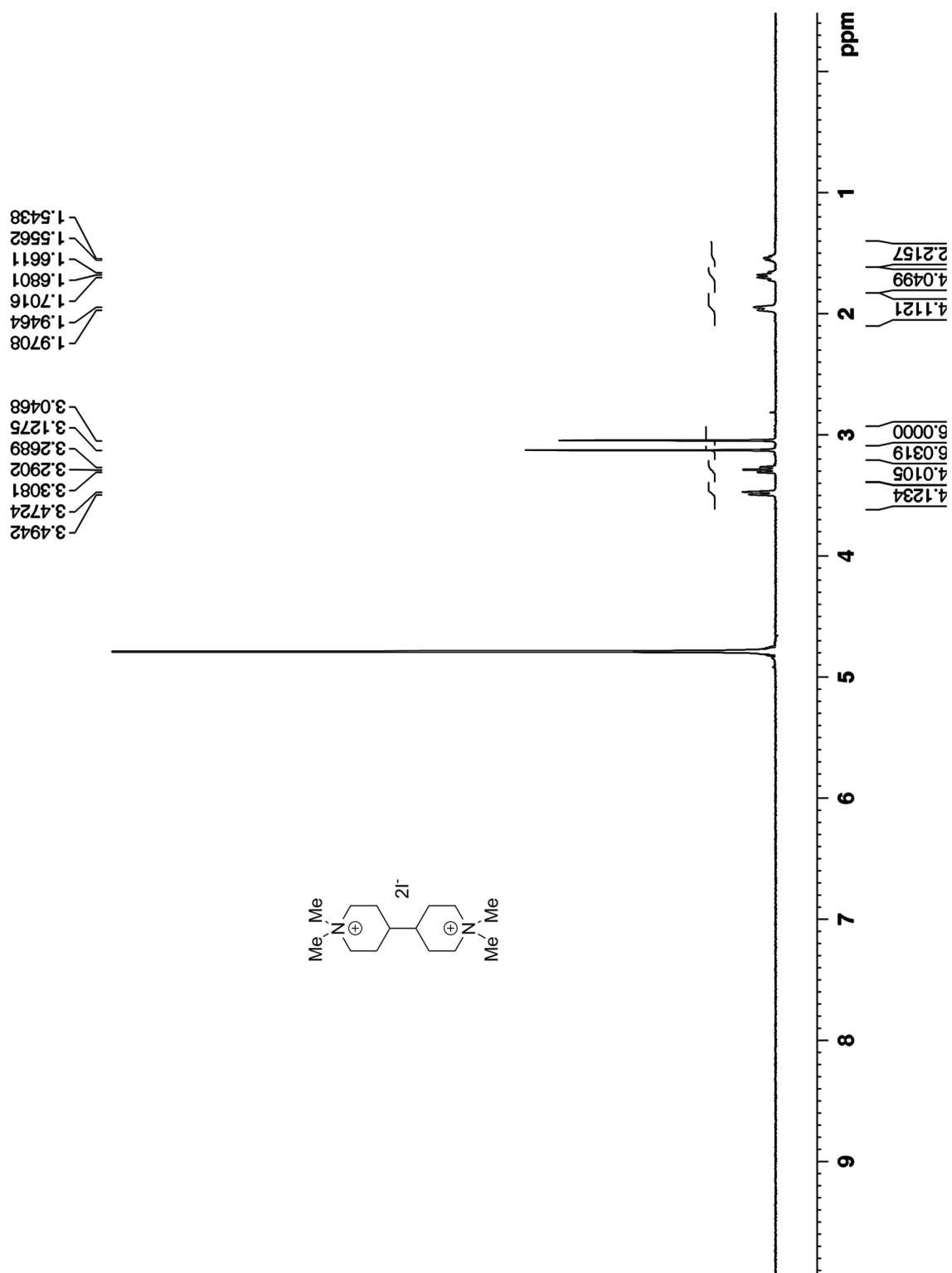


Figure S1. ¹H NMR spectrum recorded (600 MHz, D₂O, RT) for **14**.

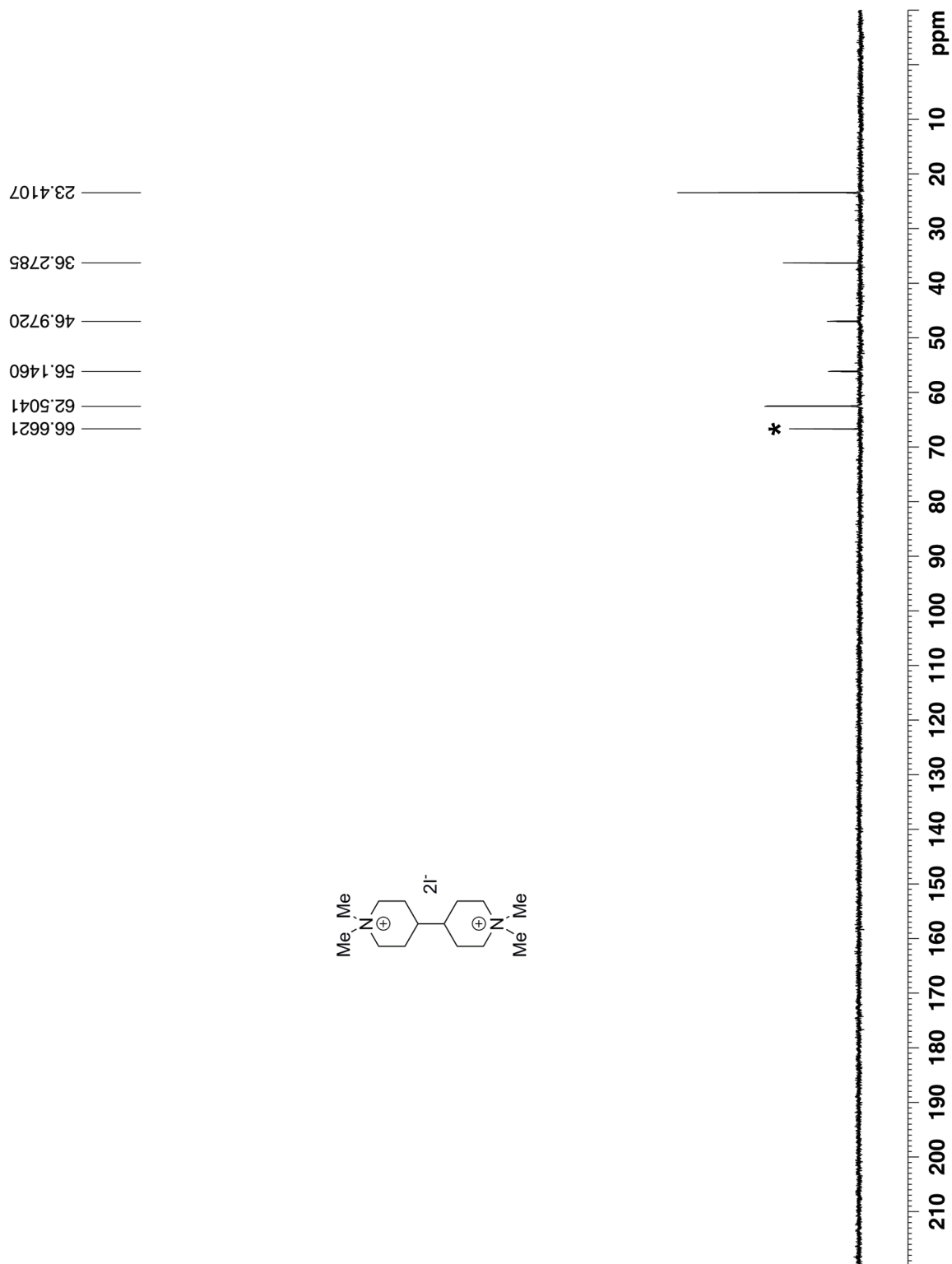


Figure S2. ^{13}C NMR spectrum recorded (125 MHz, D_2O , RT) for **14**. Internal reference = dioxane (*)

¹H NMR spectra recorded for selected CB[7]•guest complexes.

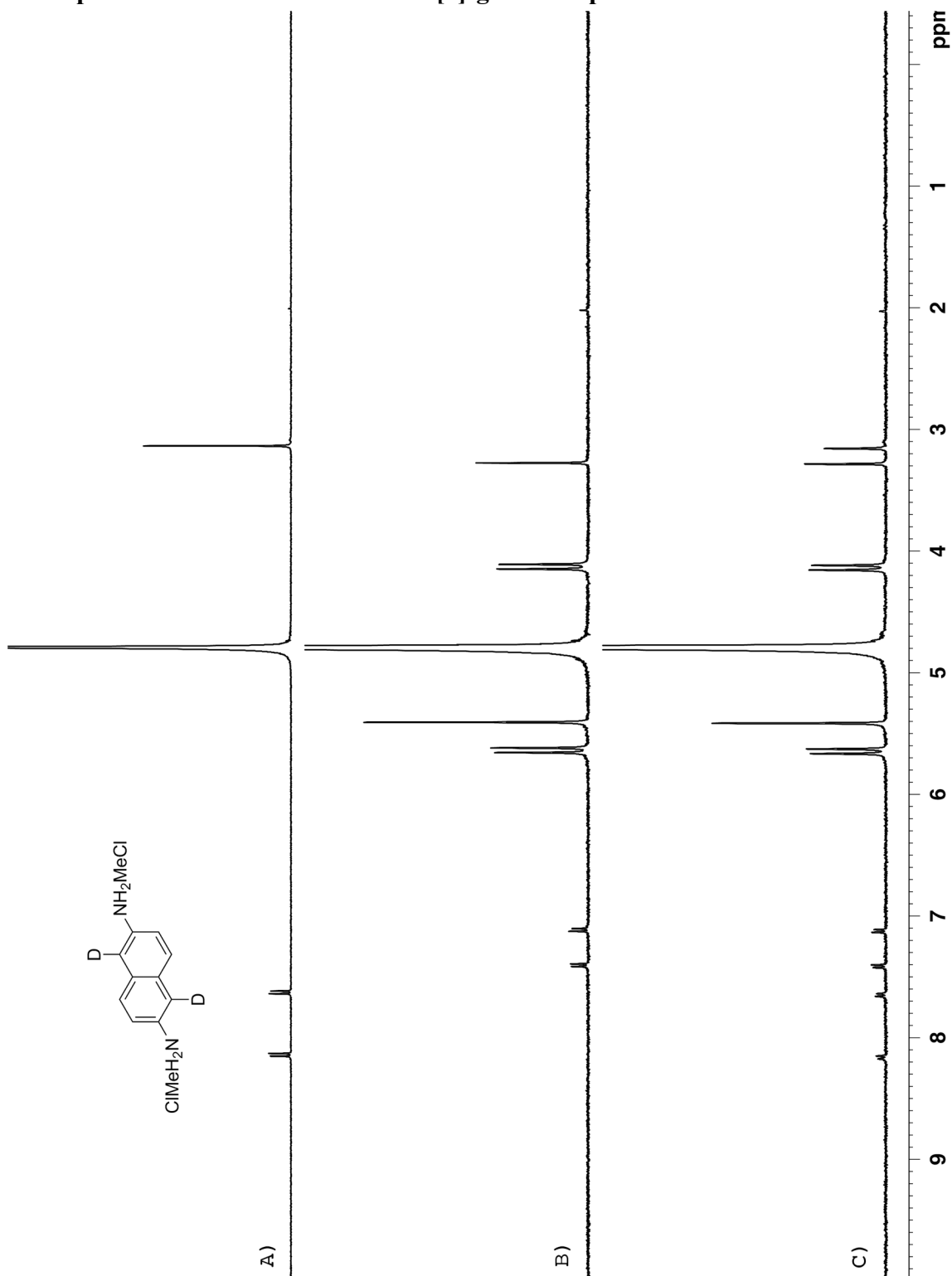


Figure S3. ¹H NMR spectra recorded (D₂O, 400 MHz, RT) for: a) **7** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **7** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **7** (0.5 mM). [Note: D-exchange happened on the 1,5-positions of guest **7** in D₂O.]

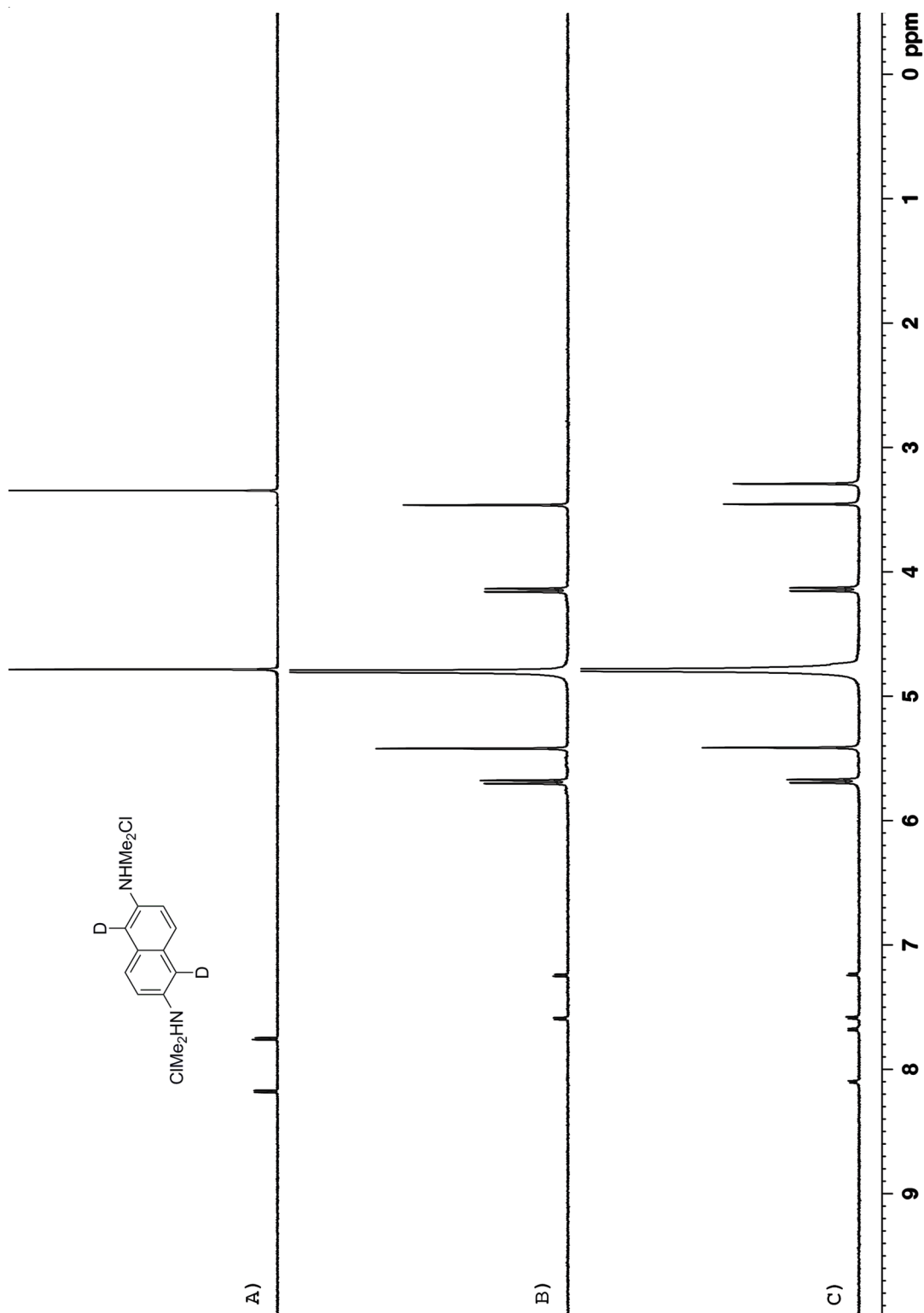


Figure S4. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **8** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **8** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **8** (0.5 mM). [Note: D-exchange happened on the 1,5-positions of guest **8** in D_2O .]



Figure S5. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **9** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **9** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **9** (0.5 mM).

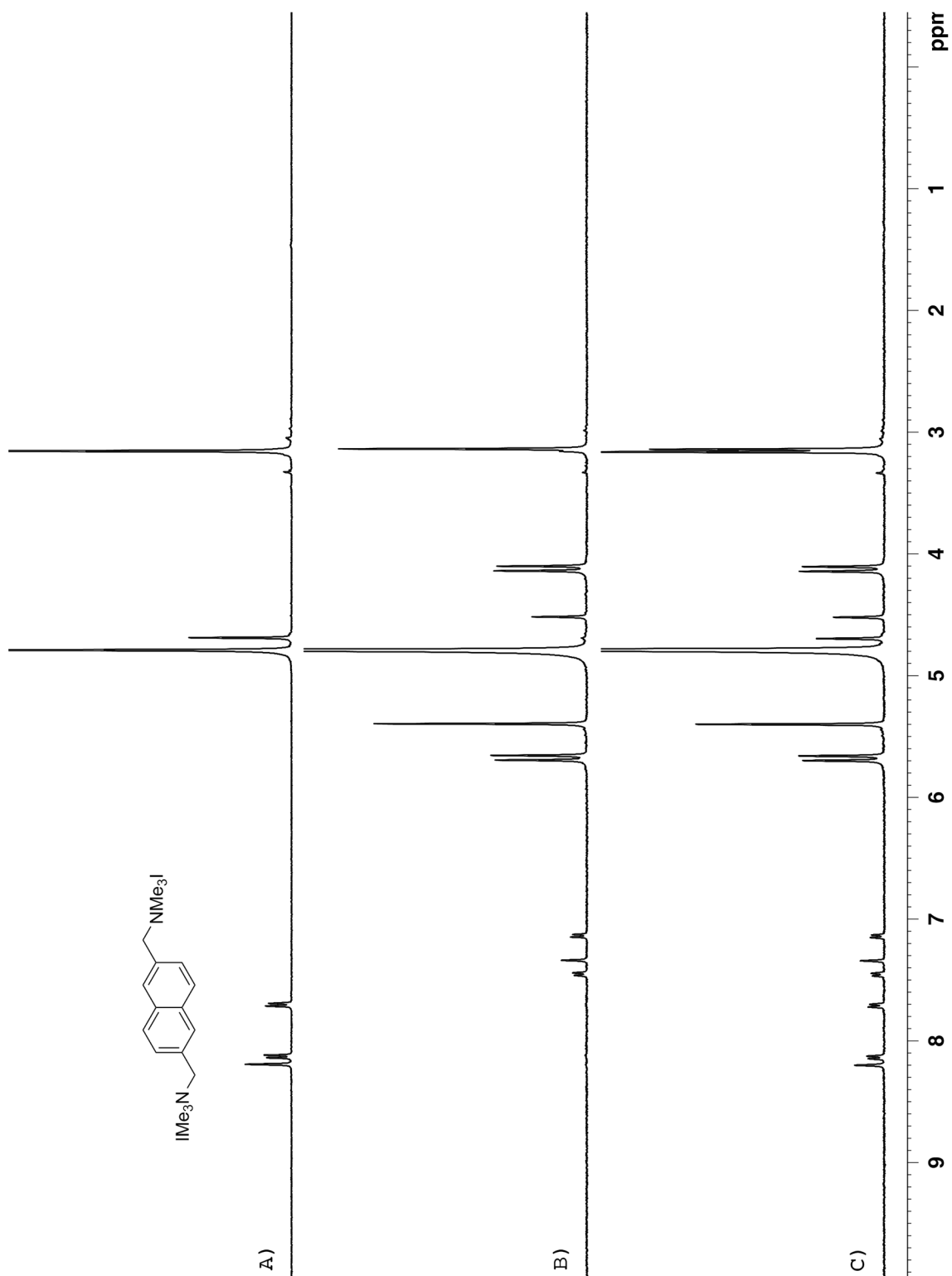


Figure S6. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **10** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **10** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **10** (0.5 mM).

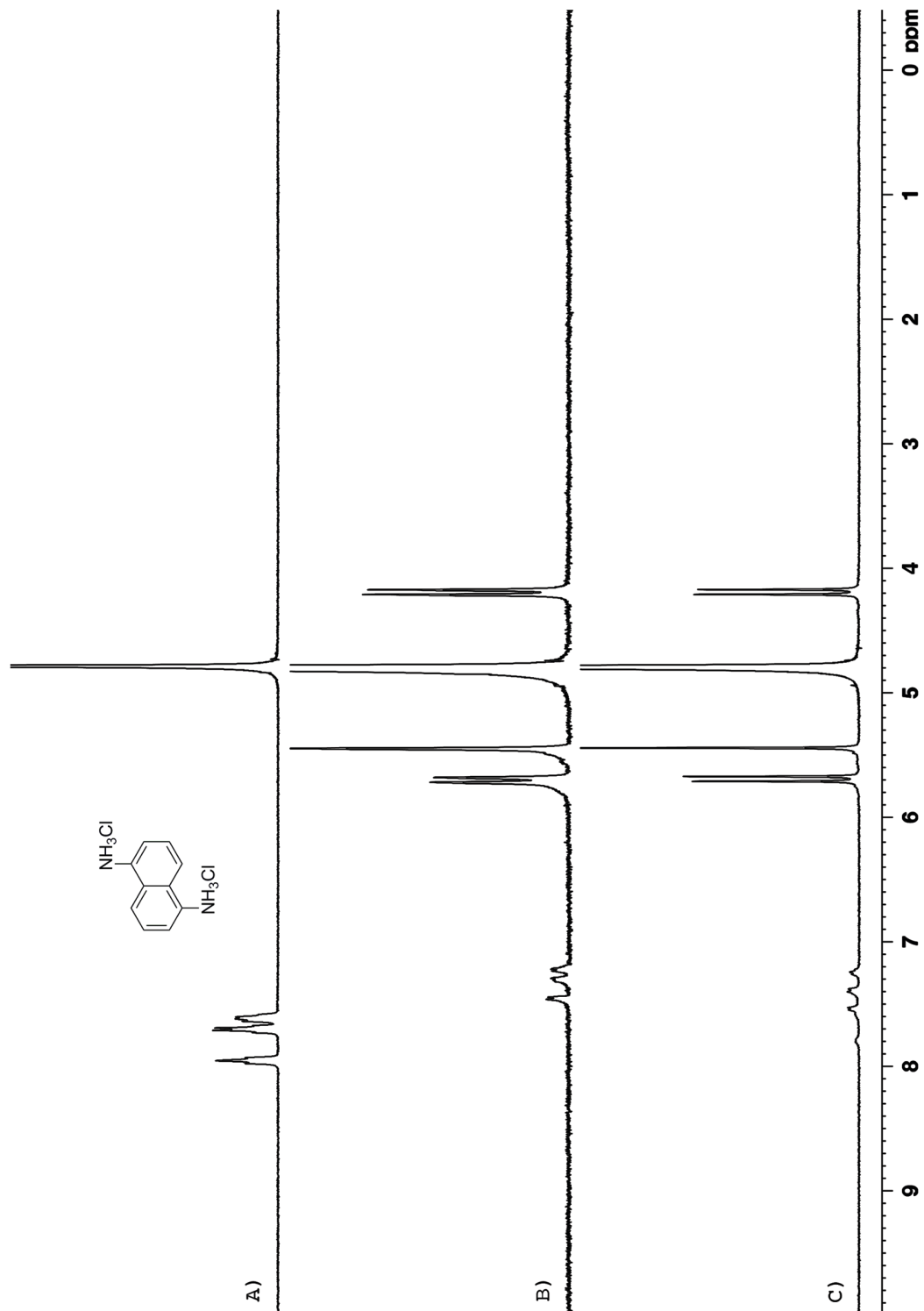


Figure S7. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **11** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **11** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **11** (0.5 mM).

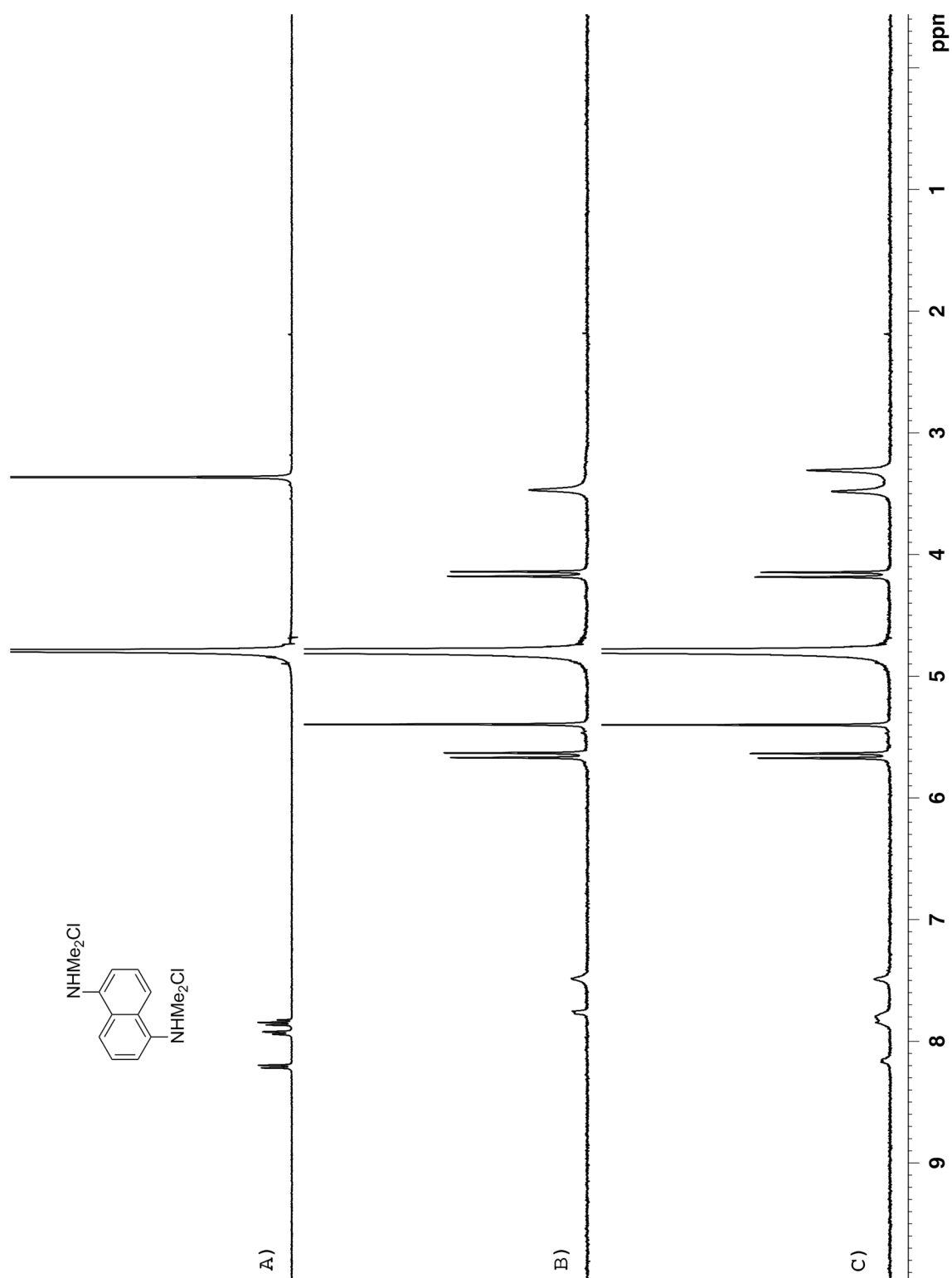


Figure S8. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **12** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **12** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **12** (0.5 mM).

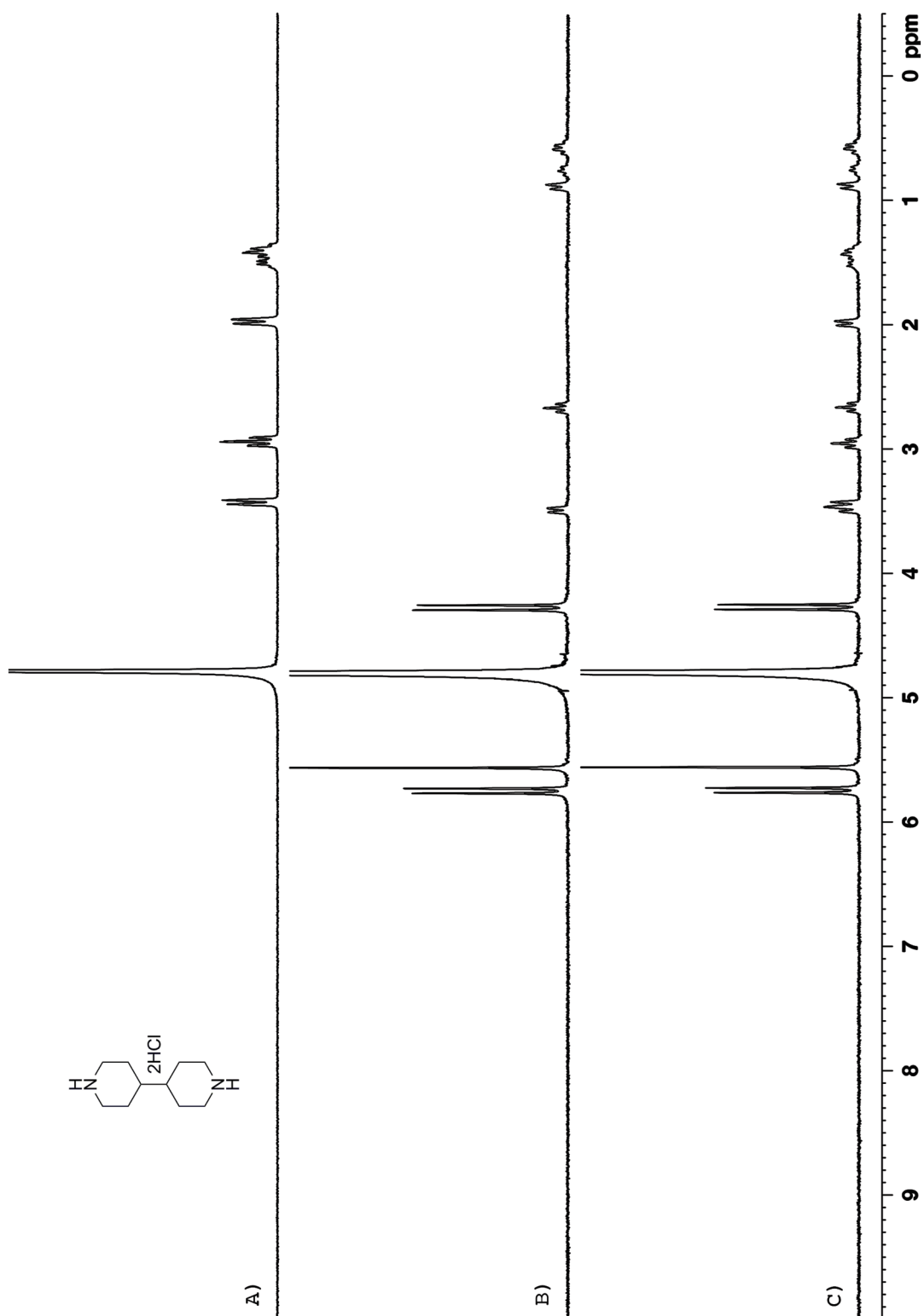


Figure S9. ^1H NMR spectra recorded (D_2O , 400 MHz, RT) for: a) **13** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **13** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **13** (0.5 mM).

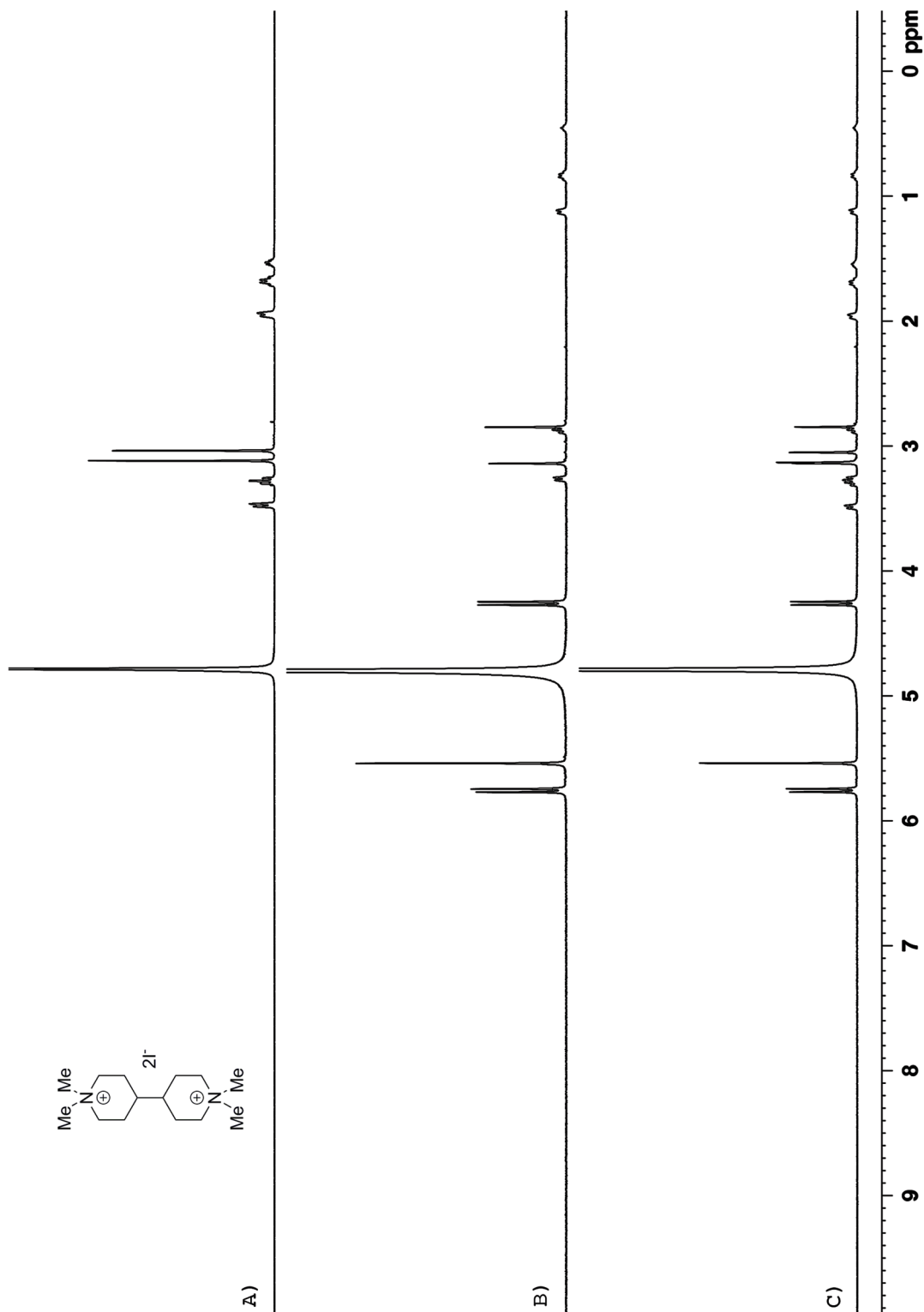


Figure S10. ¹H NMR spectra recorded (D₂O, 400 MHz, RT) for: a) **14** (0.25 mM), b) a mixture of CB[7] (0.25 mM) and **14** (0.25 mM), and c) a mixture of CB[7] (0.25 mM) and **14** (0.5 mM).

Sample Determination of K_{rel} for the Competition Between **14** and **5** for CB[7]

We use equation 1 to determine K_{rel} for the interaction of **14** and **5** for CB[7]. For this purpose, we prepared a solution containing CB[7] (0.2543 mM), **14** (0.3590 mM), **5** (24.9253 mM) and allowed it to reach equilibrium (Figure S18). Next, we determined the relative concentration of CB[7]•**14** and free **14** by integration of the appropriate resonances in the ^1H NMR spectrum (Figure S18: CB[7]•**14**: 5.56 ppm; CB[7]•**5**: 5.53 ppm). Using the concentration and the mass balance expression (equation 3) allowed us to calculate [CB[7]•**14**] (0.1251 mM) and [CB[7]•**5**] (0.1292 mM). Equation 2 is then used to calculate [**14**]_{free} (0.2339 mM) using the known value of CB[7]•**14**. Lastly, equation 4 is used to calculate [**5**]_{free} (24.7961 mM) using the known value of [CB[7]•**5**].

$$K_{rel} = ([\text{CB}[7]\cdot\mathbf{14}][\mathbf{5}]_{free}) / ([\text{CB}[7]\cdot\mathbf{5}][\mathbf{14}]_{free}) \quad (1)$$

$$[\mathbf{14}]_{Total} = 0.3590 \text{ mM} = [\mathbf{14}]_{free} + [\text{CB}[7]\cdot\mathbf{14}] \quad (2)$$

$$[\text{CB}[7]]_{Total} = 0.2543 \text{ mM} = [\text{CB}[7]\cdot\mathbf{14}] + [\text{CB}[7]\cdot\mathbf{5}] \quad (3)$$

$$[\mathbf{5}]_{Total} = 24.9253 \text{ mM} = [\mathbf{5}]_{free} + [\text{CB}[7]\cdot\mathbf{5}] \quad (4)$$

Substitution of the values of [CB[7]•**14**], [**14**]_{free}, [CB[7]•**5**], and [**5**]_{free} into equation 1 gave $K_{rel} = 102.65$. These determinations were done from independently prepared stock solutions and the average values were used in the calculations of K_a and the error analysis shown below. In preparing the solutions for the above determinations we used two methods to reach equilibrium: a) A solution of CB[7] and **14** was prepared, addition of **5** gave the final equilibrium; b) A solution of CB[7] and **5** was prepared, addition of **14** gave the final equilibrium. Under those conditions the errors in [**14**]_{free}, [**5**]_{free} are small and both [CB[7]•**14**] and [CB[7]•**5**] are kept in a good range for accurate measurement of their ratio by ^1H NMR.

Determination of K_a for CB[7]•**14** by competition of **14** and **5** for a limiting quantity of CB[7]

We used ^1H NMR competition experiments to determine $K_{rel} = 102.65$ for these two guests. Substitution of $K_{\text{CB}[7]\cdot\mathbf{5}} = (1.84 \pm 0.34) \times 10^9 \text{ M}^{-1}$ and K_{rel} into equation 5 gave $K_{\text{CB}[7]\cdot\mathbf{14}} = 1.9 \times 10^{11} \text{ M}^{-1}$ (equation 6). The uncertainty in $K_{\text{CB}[7]\cdot\mathbf{14}}$ can be determined using equation 7. Substituting $\sigma(K_{\text{CB}[7]\cdot\mathbf{5}})/K_{\text{CB}[7]\cdot\mathbf{5}} = 0.1848$ and $\sigma(K_{rel})/K_{rel} = 0.10$ [Note that we are using the even more conservative 10% error in this analysis] gives the percent error in $K_{\text{CB}[7]\cdot\mathbf{14}}$ (equation 8). Substituting eq. 6 into eq. 9 gives $\sigma(K_{\text{CB}[7]\cdot\mathbf{14}})$ (equation 9) which can be combined with eq. 6 to give a final value for $K_{\text{CB}[7]\cdot\mathbf{14}}$ (equation 10).

$$K_{\text{CB}[7]\cdot\mathbf{14}} = (K_{\text{CB}[7]\cdot\mathbf{5}})(K_{rel}) \quad (5)$$

$$K_{\text{CB}[7]\cdot\mathbf{14}} = 1.9 \times 10^{11} \text{ M}^{-1} \quad (6)$$

$$(\sigma K_{\text{CB}[7]\cdot 14}/K_{\text{CB}[7]\cdot 14})^2 = (\sigma K_{\text{CB}[7]\cdot 5}/K_{\text{CB}[7]\cdot 5})^2 + (\sigma K_{\text{rel}}/K_{\text{rel}})^2 \quad (7)$$

$$\sigma K_{\text{CB}[7]\cdot 14}/K_{\text{CB}[7]\cdot 14} = 0.2101 \text{ (21.01\%)} \quad (8)$$

$$\sigma K_{\text{CB}[7]\cdot 14} = (0.2101) \times (1.9 \times 10^{11} \text{ M}^{-1}) = 0.4 \times 10^{11} \quad (9)$$

$$K_{\text{CB}[7]\cdot 14} = (1.9 \pm 0.4) \times 10^{11} \text{ M}^{-1} \quad (10)$$

Selected ^1H NMR spectra from the K_a and K_{rel} measurements

The following spectra are representative examples of those acquired during the determination of the various K_a and K_{rel} values. The resonance at ≈ 1.9 ppm is due to residual H-atoms present in the $\text{CD}_3\text{CO}_2\text{D}$ used to make the buffer. The integral is determined by deconvolution using MestRe Nova.

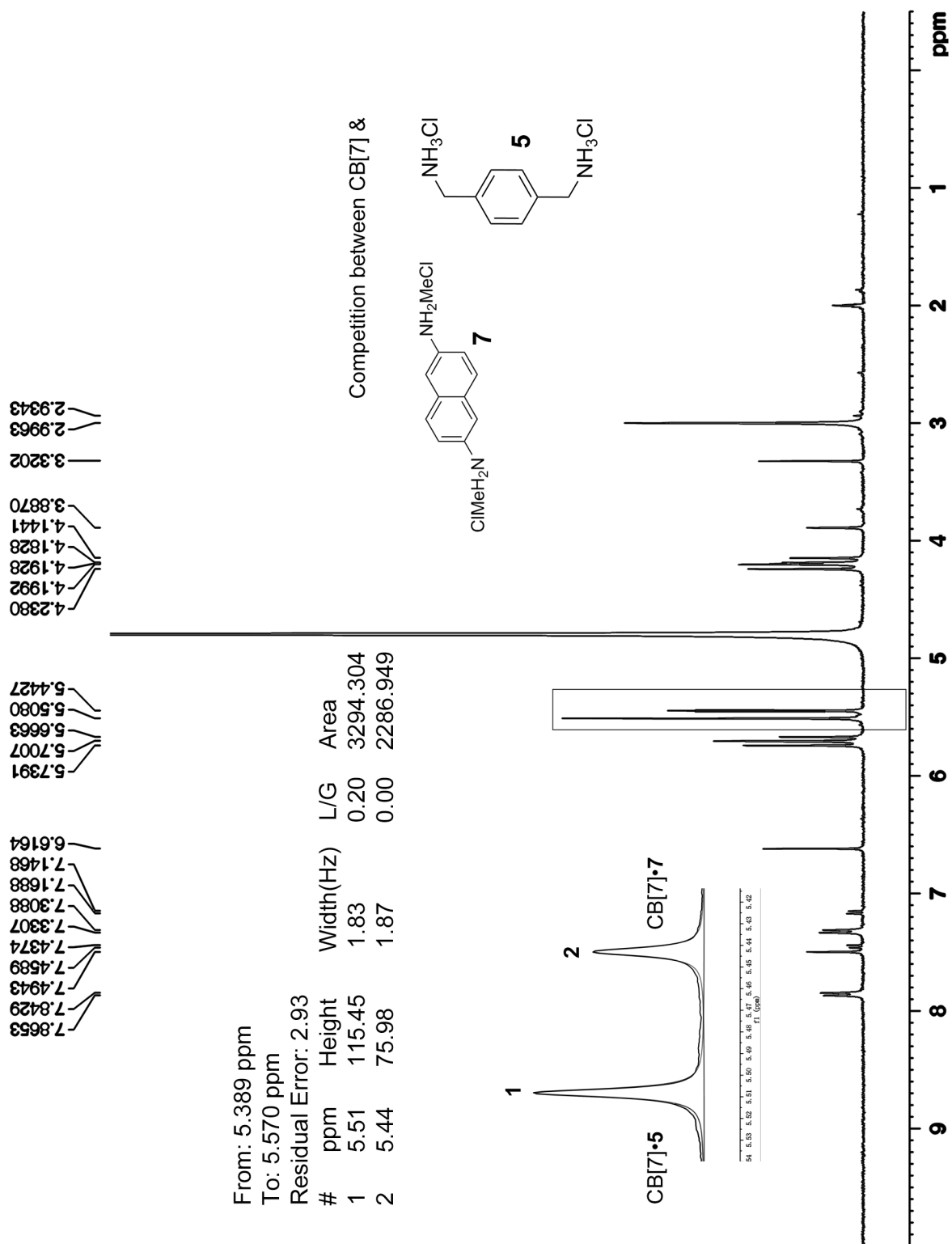


Figure S11. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, $\text{pD} = 4.74$, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{7}$ and $\text{CB}[7]\cdot\mathbf{5}$. $[\text{CB}[7]]_{\text{Total}} = 0.2486$ mM, $[\mathbf{7}]_{\text{Total}} = 0.6446$ mM, $[\mathbf{5}]_{\text{Total}} = 0.2563$ mM, $K_{\text{rel}} = 1.40 \times 10^{-1}$.

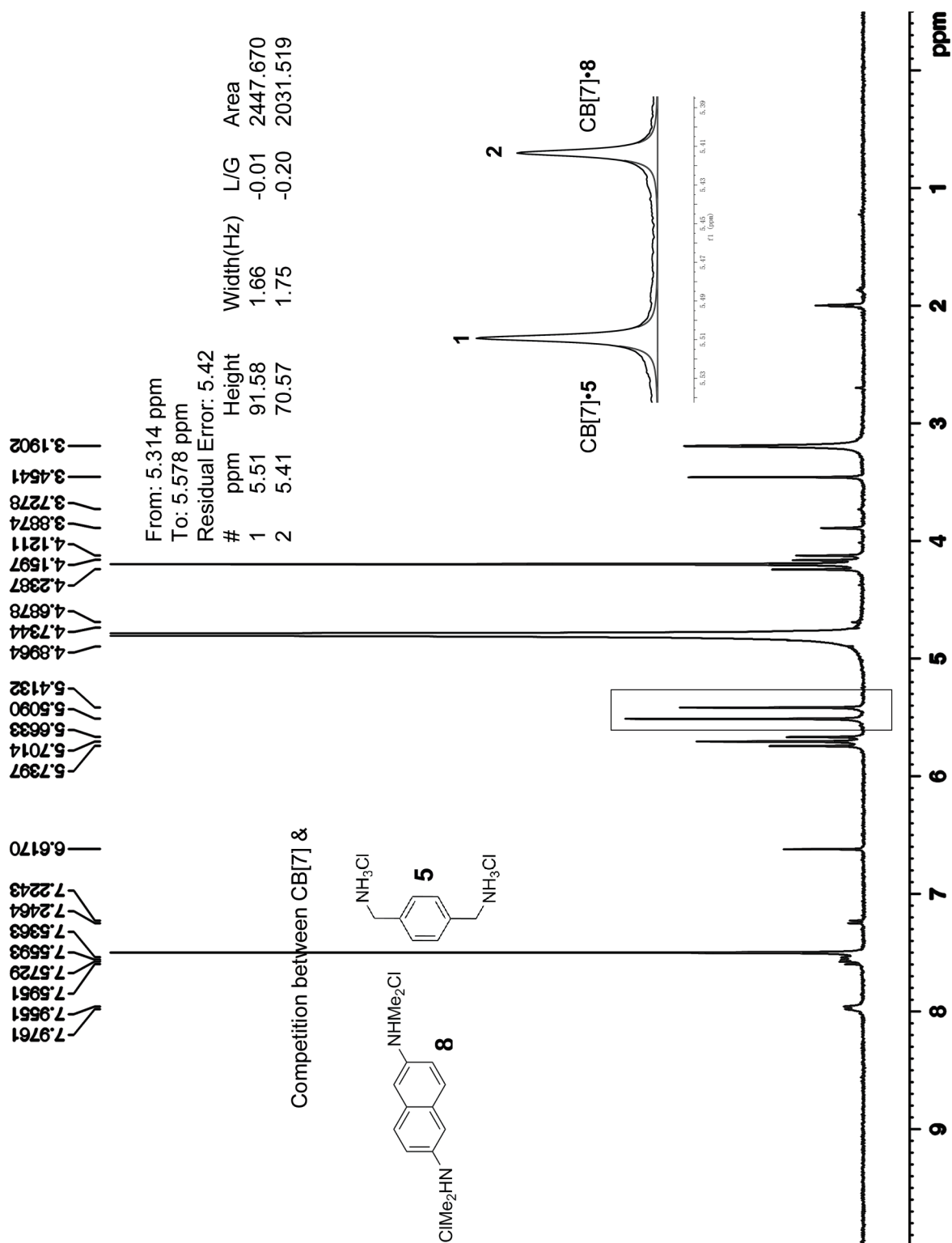


Figure S12. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, pD = 4.74, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{8}$ and $\text{CB}[7]\cdot\mathbf{5}$. $[\text{CB}[7]]_{\text{Total}} = 0.2486\text{mM}$, $[\mathbf{8}]_{\text{Total}} = 0.4019\text{mM}$, $[\mathbf{5}]_{\text{Total}} = 0.5980\text{mM}$, $K_{\text{rel}} = 1.33$.

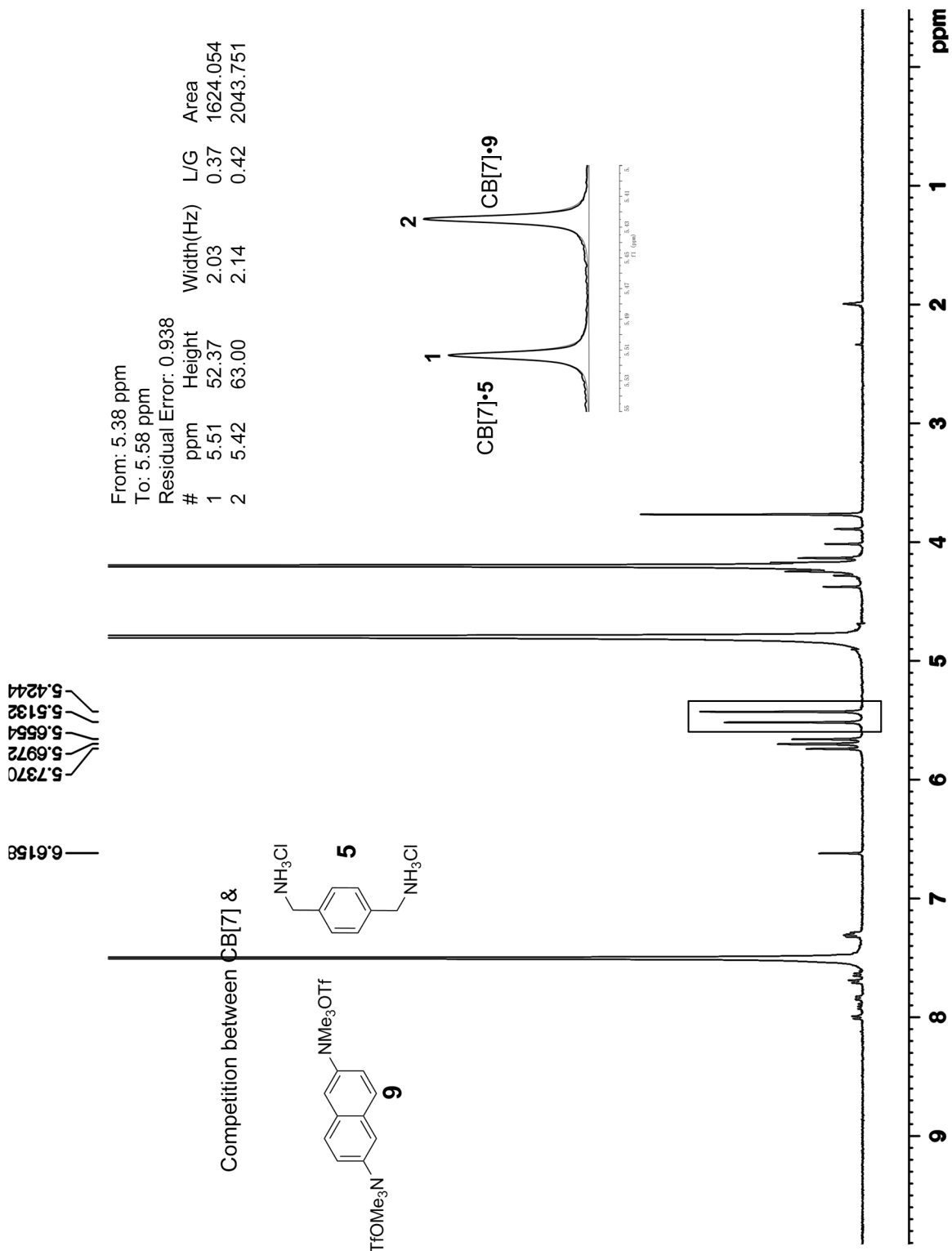


Figure S13. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, $\text{pD} = 4.74$, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{9}$ and $\text{CB}[7]\cdot\mathbf{5}$. $[\text{CB}[7]]_{\text{Total}} = 0.2312$ mM, $[\mathbf{9}]_{\text{Total}} = 0.2612$ mM, $[\mathbf{5}]_{\text{Total}} = 9.7852$ mM, $K_{\text{rel}} = 91.99$.

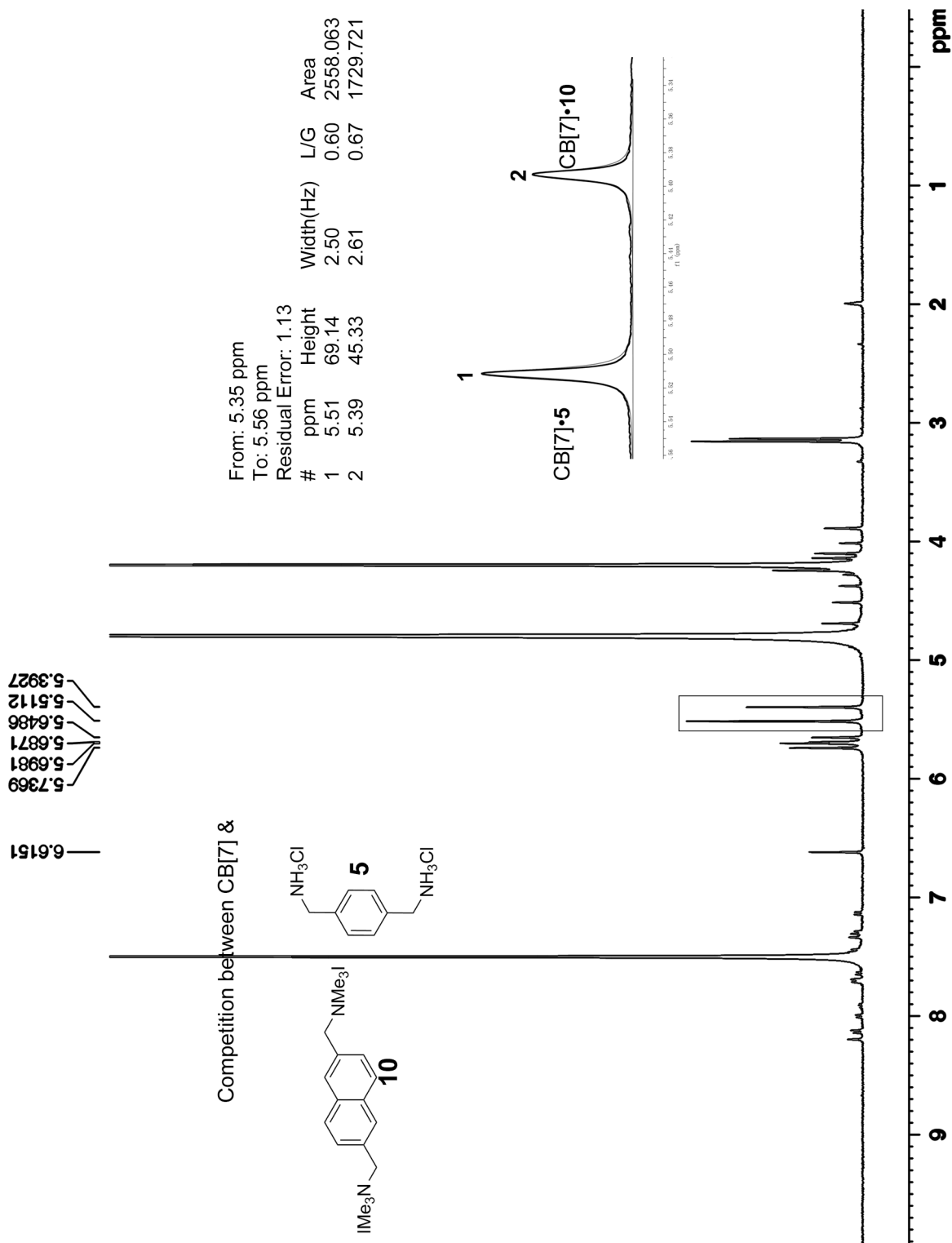


Figure S14. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, pD = 4.74, rt) used in the determination of K_{rel} for CB[7]•**10** and CB[7]•**5**. $[\text{CB}[7]]_{\text{Total}} = 0.2543$ mM, $[\mathbf{10}]_{\text{Total}} = 0.4181$ mM, $[\mathbf{5}]_{\text{Total}} = 6.8069$ mM, $K_{\text{rel}} = 14.25$.

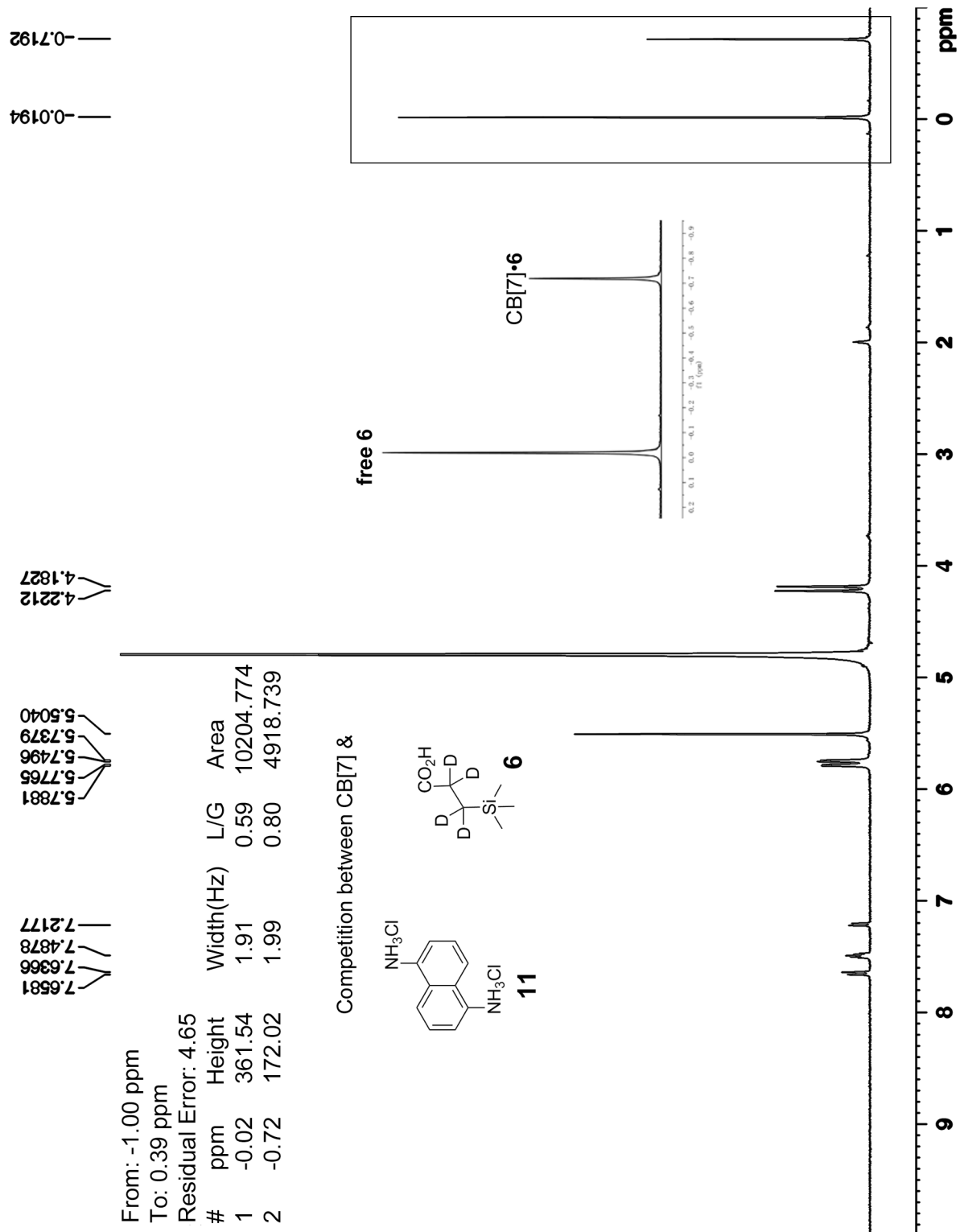


Figure S15. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, pD = 4.74, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{11}$ and $\text{CB}[7]\cdot\mathbf{6}$. $[\text{CB}[7]]_{\text{Total}} = 0.2486$ mM, $[\mathbf{11}]_{\text{Total}} = 0.9113$ mM, $[\mathbf{6}]_{\text{Total}} = 0.3720$ mM, $K_{\text{rel}} = 3.38 \times 10^{-1}$.

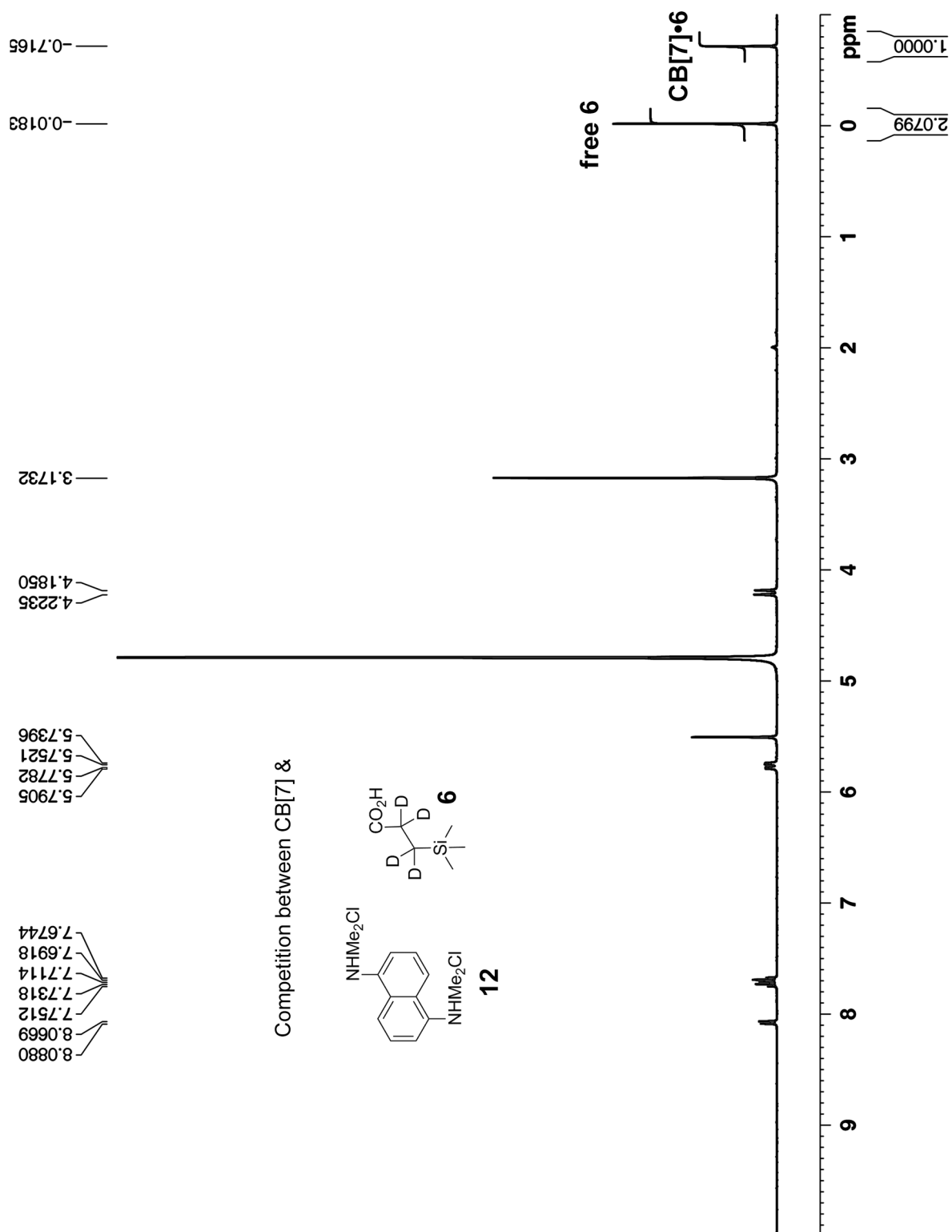


Figure S16. One of the ^1H NMR spectra (400 MHz, D_2O , 50 mM NaOAc buffer, $\text{pD} = 4.74$, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{12}$ and $\text{CB}[7]\cdot\mathbf{6}$. $[\text{CB}[7]]_{\text{Total}} = 0.2543$ mM, $[\mathbf{12}]_{\text{Total}} = 0.8998$ mM, $[\mathbf{6}]_{\text{Total}} = 0.3720$ mM, $K_{\text{rel}} = 3.62 \times 10^{-1}$.

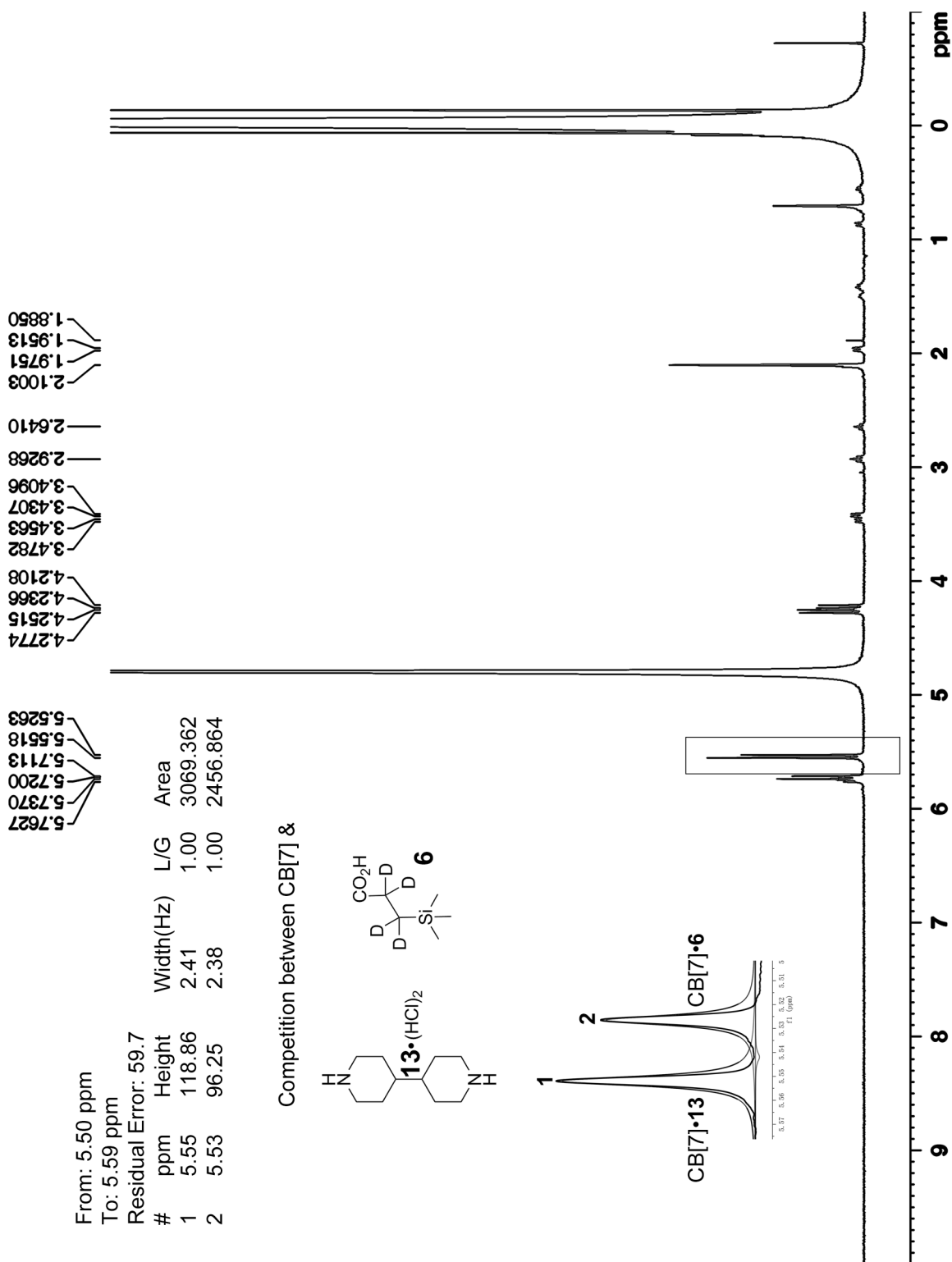


Figure S17. One of the ^1H NMR spectra (600 MHz, D_2O , 50 mM NaOAc buffer, pD = 4.74, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{13}$ and $\text{CB}[7]\cdot\mathbf{6}$. $[\text{CB}[7]]_{\text{Total}} = 0.2543$ mM, $[\mathbf{13}]_{\text{Total}} = 0.3570$ mM, $[\mathbf{6}]_{\text{Total}} = 134.8447$ mM, $K_{\text{rel}} = 779.45$.

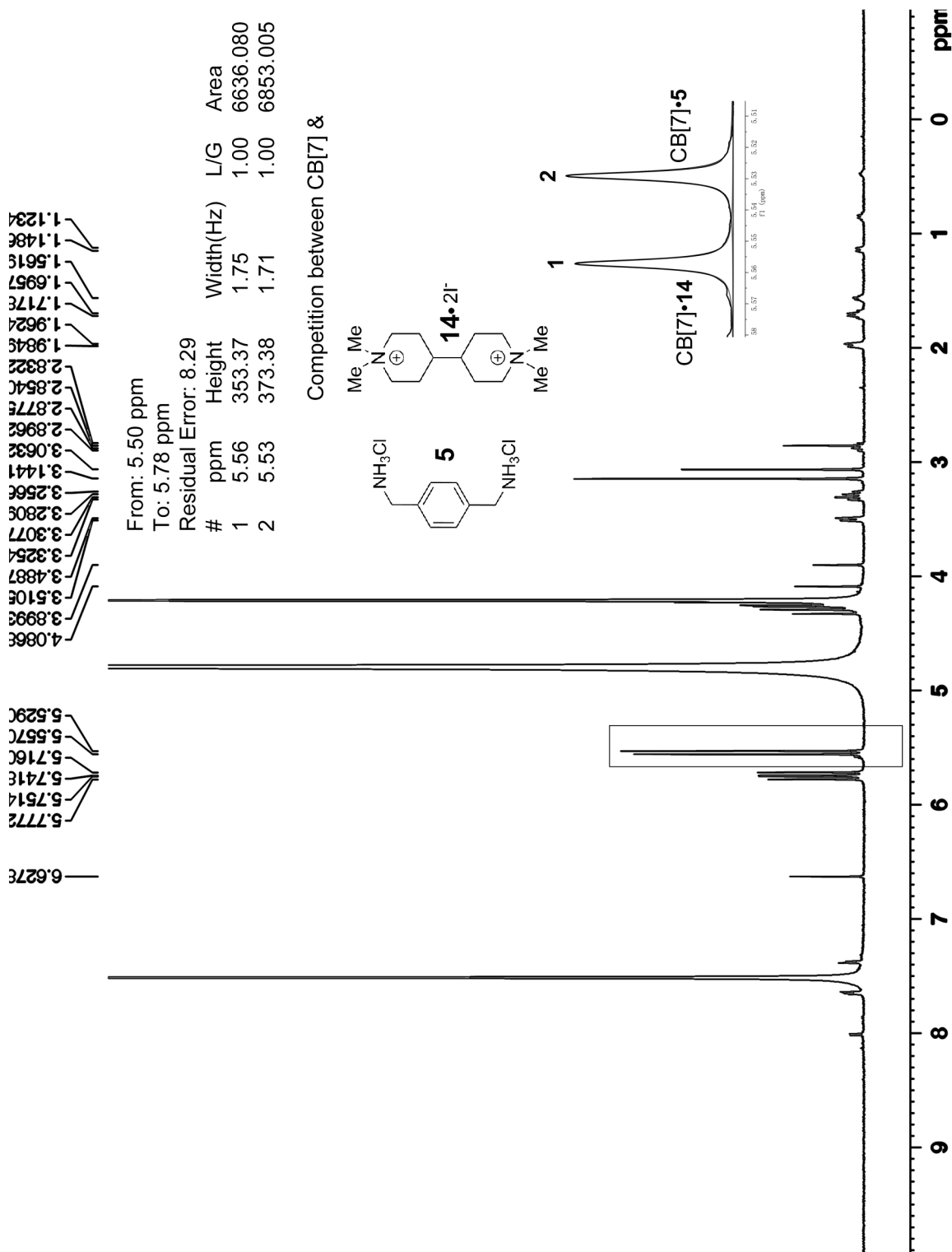


Figure S18. One of the ^1H NMR spectra (600 MHz, D_2O , 50 mM NaOAc buffer, pD = 4.74, rt) used in the determination of K_{rel} for $\text{CB}[7]\cdot\mathbf{14}$ and $\text{CB}[7]\cdot\mathbf{5}$. $[\text{CB}[7]]_{\text{Total}} = 0.2543$ mM, $[\mathbf{14}]_{\text{Total}} = 0.3590$ mM, $[\mathbf{5}]_{\text{Total}} = 24.9253$ mM, $K_{\text{rel}} = 102.65$

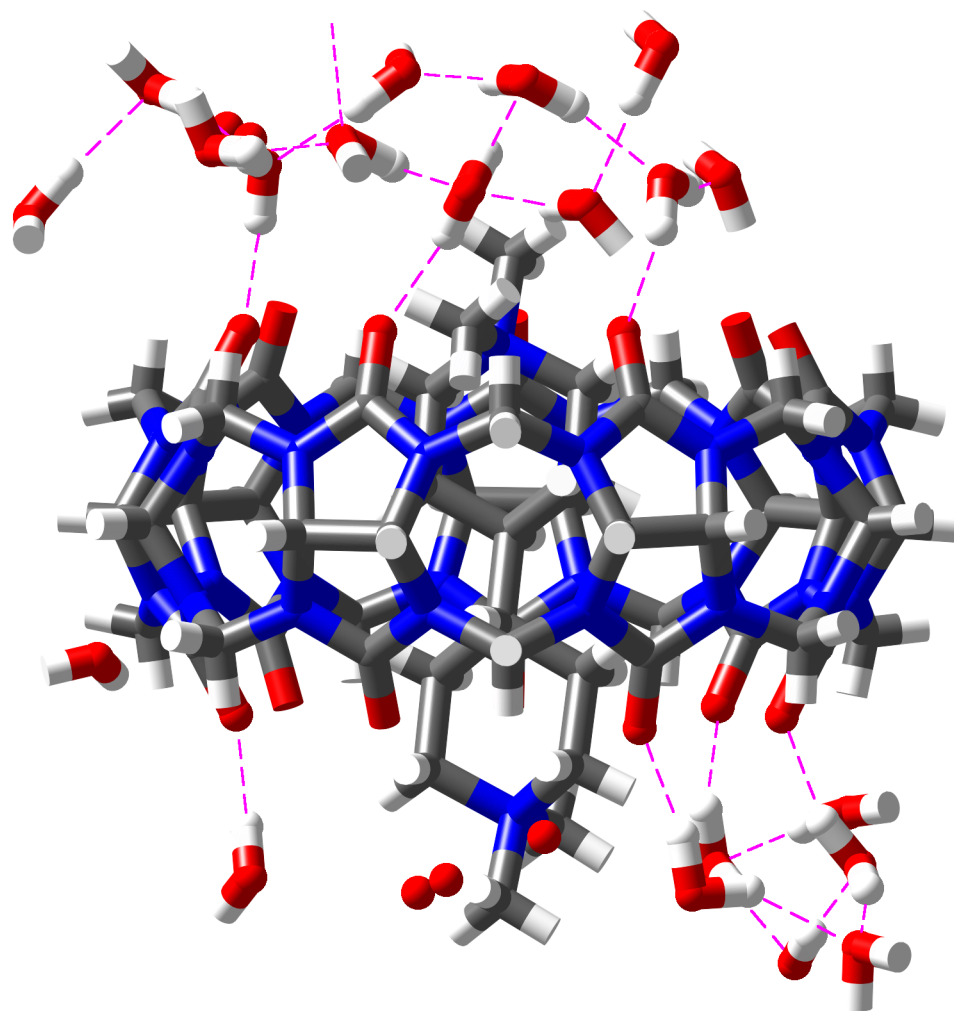


Figure S19. Illustration of the solvating H₂O molecules well ordered around the ureidyl C=O groups from the structure of CB[7]•14.

Coordinates of the minimized geometry of CB[7]•**1b**.

E: -2994513.11649975 kcal/mol

N	1.957286589	6.799696985	9.054726290
C	1.440571357	8.166743555	8.939254611
H	0.731770285	8.375574803	9.768277989
N	2.444340737	9.222446739	8.852886756
C	1.629648532	6.010253583	7.951921149
O	1.854795438	4.803727951	7.829881308
C	2.458969676	9.857390681	7.608512229
O	3.153473619	10.821365521	7.291965216
N	0.970751958	6.818037516	7.025894852
C	0.769183271	8.183314049	7.513949778
H	-0.314947581	8.423652930	7.535134416
N	1.505961214	9.226254765	6.804027461
C	0.305952004	6.269175630	5.849424224
H	0.317901021	5.169414222	5.951371409
H	-0.742975249	6.633438668	5.830819724
C	1.092577755	9.778505018	5.521353090
H	1.575996601	10.767116691	5.424741369
H	-0.011898729	9.897074233	5.517914368
N	0.940149543	6.586204930	4.575476128
C	0.733934373	7.847417166	3.859395363
H	-0.349762272	8.087504761	3.816840108
N	1.486065180	8.995443052	4.358094862
C	1.533088617	5.606582336	3.776257356
O	1.715776805	4.428121201	4.088050498
C	2.439438714	9.455602344	3.444013729
O	3.145130422	10.453987932	3.572018523
N	1.849429713	6.193600589	2.549708613
C	1.375041184	7.574855248	2.447388978
H	0.654972673	7.667081926	1.606560786
N	2.410117182	8.599916299	2.339860864
C	2.314343060	5.416161051	1.407452407
H	1.660493141	5.630782711	0.535954643
H	2.229843216	4.349945011	1.683197243
C	3.109968581	8.917339455	1.102014012
H	3.498158273	9.946507014	1.204144840
H	2.388481395	8.868154794	0.258856955
N	3.701838422	5.652810824	1.024641588
C	4.135140525	6.753786162	0.160920006

H	3.476640899	6.817547849	-0.731377388
N	4.248205181	8.061655277	0.800802383
C	4.690719106	4.682375451	1.188407643
O	4.558388392	3.603093573	1.768491713
C	5.562814348	8.535683647	0.836513831
O	5.926769176	9.641217539	1.232659338
N	5.844487274	5.132505844	0.546801397
C	5.628419370	6.385321149	-0.181437129
H	5.810767878	6.230071443	-1.266119177
N	6.381597414	7.540288145	0.297129791
C	7.009242797	4.274871984	0.361227737
H	6.722261230	3.259710003	0.688263211
H	7.274292503	4.258528934	-0.717044260
C	7.788175290	7.770221240	0.000307771
H	7.974081403	8.851432681	0.129807942
H	7.986391887	7.476909104	-1.052318818
N	8.187567651	4.662441194	1.127610260
C	9.136194455	5.682751960	0.676477194
H	9.403858810	5.507483420	-0.387232877
N	8.723800127	7.070461421	0.870170218
C	8.684744232	3.893964997	2.182801985
O	8.138365541	2.909163813	2.685043422
C	9.529471649	7.750297087	1.787153481
O	9.463887625	8.945699569	2.066751120
N	9.926356236	4.422575727	2.543845297
C	10.347912374	5.517872391	1.667085673
H	11.301778912	5.253428519	1.163090263
N	10.455503149	6.833123677	2.292749287
C	10.833421260	3.737652641	3.458754019
H	10.403684015	2.741324489	3.664879936
H	11.820016034	3.622414650	2.961926050
C	11.581869140	7.249966786	3.115463654
H	11.585367949	8.354688493	3.121666896
H	12.521951036	6.872802251	2.659323611
N	11.026844645	4.397324255	4.744381058
C	11.965876464	5.499849537	4.959749456
H	12.952151495	5.251215227	4.513022975
N	11.522729263	6.814662984	4.503922037
C	10.568894301	3.843614956	5.940868077
O	9.871902888	2.834184057	6.053232585
C	11.345257507	7.718820620	5.554662007

O	11.067511574	8.911735890	5.447771734
N	11.074073767	4.614561319	6.989516405
C	12.004030725	5.648275338	6.527688342
H	13.010089255	5.476614635	6.966235605
N	11.587115721	7.030007409	6.746307239
C	10.937605032	4.208679633	8.383723221
H	10.516325589	3.187678952	8.385927245
H	11.943067999	4.197839476	8.854971335
C	11.673258642	7.711768815	8.029618387
H	11.677714887	8.796251687	7.819592832
H	12.621563849	7.420498953	8.528840140
N	10.053882082	5.045697850	9.186905477
C	10.481666582	6.295159308	9.818790343
H	11.447008326	6.142770155	10.346675357
N	10.564367571	7.458018146	8.939122698
C	8.821311509	4.595979862	9.663876315
O	8.269515144	3.534237754	9.364708399
C	9.629834182	8.446259126	9.258658338
O	9.534970688	9.554249818	8.735199632
N	8.339457712	5.549586597	10.563253402
C	9.285454091	6.646917153	10.780190775
H	9.574200750	6.693286536	11.851625329
N	8.852704077	7.962489794	10.315914176
C	7.183873544	5.304822167	11.419315119
H	7.477143533	5.488056207	12.474676003
H	6.900149763	4.245204984	11.290987723
C	7.929755266	8.818845078	11.047521795
H	8.092164714	9.850708926	10.687941649
H	8.162669294	8.756352355	12.131835089
N	6.003605189	6.104544953	11.113004727
C	5.802466562	7.476893017	11.583153126
H	6.033867895	7.544086974	12.667475785
N	6.519235270	8.515641283	10.848364452
C	4.835375458	5.538112573	10.602074506
O	4.692860495	4.368385058	10.240224385
C	5.661783909	9.393863204	10.178131550
O	5.993570959	10.404966838	9.563192142
N	3.845698337	6.522187118	10.607417700
C	4.291599965	7.764704775	11.241858338
H	3.667337420	7.980366677	12.134954048
N	4.355482074	8.937670876	10.375258814

C	2.452640604	6.224291194	10.300916021
H	2.368349997	5.126744027	10.210212908
H	1.814714099	6.581427872	11.136851857
C	3.194990894	9.731059991	9.992188975
H	2.512614562	9.812619242	10.864316096
H	3.566808444	10.732559861	9.711346693
C	5.854103325	5.034899031	5.895151520
C	4.800313789	2.938814311	4.786798112
H	5.365646679	3.180462706	3.875358873
H	3.796461377	3.387889742	4.738365055
H	4.710677118	1.842953041	4.879939167
C	6.822875303	2.640052702	6.137326750
H	6.539856912	1.589688823	6.322323878
H	7.418549696	3.009656139	6.985314514
H	7.399884531	2.705815805	5.203979354
C	4.685893931	3.136811410	7.229845090
H	3.772810761	3.752756556	7.223743022
H	5.257398540	3.325903325	8.149921230
H	4.408859719	2.070037765	7.178275035
C	6.378030684	5.555858556	7.257383959
H	7.292559614	5.011224392	7.550079955
H	5.629640392	5.387532039	8.049658635
C	4.561492940	5.801371962	5.511903289
H	3.757031946	5.608621368	6.243791237
H	4.195834814	5.467165186	4.525295186
C	6.928275326	5.294539439	4.805112825
H	6.583266962	4.926877467	3.821307304
H	7.868086099	4.767141675	5.044377687
C	6.682974151	7.077121355	7.163727724
H	7.055844708	7.409165088	8.151504634
C	4.858524462	7.327983230	5.439857287
H	3.912895578	7.844180323	5.186189932
C	7.220556909	6.822155370	4.713017254
H	7.988110291	6.972930876	3.929778479
C	5.921072147	7.580130468	4.340295892
H	6.118978170	8.665155883	4.227840290
H	5.539761827	7.224930696	3.361494910
C	7.758644099	7.323027231	6.077727227
H	8.022530646	8.398494260	6.025471053
H	8.690110873	6.782789814	6.343683648
C	5.378457397	7.832354593	6.808921936

H	5.555116135	8.926378820	6.780262215
H	4.616406484	7.656268096	7.594732143
N	5.540309514	3.442974066	6.011494061

Coordinates of the minimized geometry of CB[7]•14.

E: -3054875.68327804 kcal/mol

N	22.556730482	22.367650304	25.461006285
C	22.563136639	21.081868247	26.304861912
H	23.597608915	20.968691332	26.671733841
H	22.338095333	20.241680790	25.625990789
C	21.575631742	21.116379705	27.474583544
H	21.730855742	20.164367054	28.015520779
H	20.531373270	21.092461505	27.102771436
C	21.797110650	22.331867688	28.407641692
H	22.818215651	22.237224452	28.842124415
C	21.773717924	23.625226623	27.557138461
H	20.747881087	23.837791018	27.194413657
H	22.075914933	24.503363430	28.157845161
C	22.758742455	23.580162313	26.385611477
H	22.669469462	24.486683811	25.763010234
H	23.797019396	23.508644095	26.752596850
C	23.724112362	22.308579831	24.497908777
H	23.597890184	21.431590631	23.840932423
H	24.657645906	22.219454087	25.077862476
H	23.734892517	23.233961321	23.897640036
C	21.274342996	22.492963675	24.662087475
H	20.399604124	22.549339227	25.325211018
H	21.183747500	21.607754977	24.010985630
H	21.333010279	23.411329905	24.054869665
N	20.165378662	22.327540919	32.579735551
C	19.924800770	21.114661016	31.670916831
H	20.049740270	20.213694596	32.294966463
H	18.861921549	21.170380937	31.374662214
C	20.844461552	21.076140379	30.445759151
H	21.893018381	20.870321312	30.747358938
H	20.523932652	20.198056549	29.852232254
C	20.789787297	22.371025907	29.593111037
H	19.761881714	22.458024672	29.169974281
C	21.026045220	23.592816438	30.519555007
H	20.834116938	24.540293058	29.979614581

H	22.092635481	23.629884297	30.825883393
C	20.107473368	23.614896518	31.746494983
H	20.360664053	24.449716387	32.421849733
H	19.048707662	23.733451955	31.453811116
C	19.055697815	22.376589529	33.610310254
H	19.085516073	21.448438180	34.205520628
H	18.089883474	22.463515201	33.085097977
H	19.217630541	23.250903129	34.262861321
C	21.498360378	22.207879207	33.288827554
H	21.639764136	23.084993996	33.939028624
H	22.308081851	22.185903374	32.550200876
H	21.517569780	21.267394095	33.860931946
N	26.325841998	23.032976601	29.820002863
C	26.692113242	22.611322399	31.171431181
H	27.716297040	22.963056357	31.417087372
N	25.758302043	22.996024790	32.230601402
C	26.004975652	21.957403651	28.988863053
O	25.702405030	22.025745923	27.794037602
C	25.166413757	21.894125591	32.848889447
O	24.441640660	21.921934736	33.844700875
N	26.124077623	20.787593593	29.743016909
C	26.556817866	21.044879473	31.116418292
H	27.505309656	20.506601555	31.324848595
N	25.570983549	20.752248146	32.157159603
C	26.191017376	19.465355631	29.130161108
H	27.106848298	18.955089918	29.497349107
H	26.258499738	19.604773486	28.036689508
C	25.253042622	19.410007540	32.626054069
H	26.194318580	18.834842527	32.752719575
H	24.752709423	19.524489937	33.604060263
N	25.036963709	18.615278214	29.378518472
C	24.825775218	17.863792121	30.617978475
H	25.744045385	17.301344065	30.888658818
N	24.360504776	18.649163583	31.759159054
C	24.197063263	18.197291232	28.346056967
O	24.233250452	18.586095020	27.177702996
C	23.037571835	18.361490294	32.106515054
O	22.408152680	18.852053497	33.045410654
N	23.336130936	17.232048812	28.867046990
C	23.596365913	16.942182334	30.275231230
H	23.797327002	15.858895541	30.412510090

N	22.569153092	17.389335974	31.218892351
C	22.396282488	16.494078678	28.034522440
H	22.472027280	15.414341213	28.277876972
H	22.691256604	16.661974511	26.983550514
C	21.324694751	16.664554183	31.447551093
H	21.530775708	15.575170710	31.388317243
H	20.972442122	16.921567490	32.462397875
N	21.005232642	16.910628005	28.164014932
C	20.097613186	16.408778912	29.192512396
H	20.164862941	15.301953604	29.254812835
N	20.247440495	16.997378334	30.525686706
C	20.345063050	17.630587020	27.165201883
O	20.850526405	18.081909258	26.137977116
C	19.100791602	17.671301732	30.945575120
O	18.904416581	18.145205447	32.065980963
N	18.997468607	17.712990805	27.526636221
C	18.686923940	16.929944420	28.724097743
H	17.972434658	16.116838929	28.475398222
N	18.203787733	17.688055432	29.877355932
C	17.986099819	18.205287286	26.599878252
H	17.197529850	17.433040301	26.477597142
H	18.492734508	18.379293271	25.633924147
C	16.843521240	18.189758561	30.017907808
H	16.134879426	17.425129377	29.637057056
H	16.670876711	18.356757488	31.095991007
N	17.356357426	19.459188409	26.989270408
C	16.232243199	19.552340130	27.919510473
H	15.454135462	18.803949301	27.660877016
N	16.579265727	19.452200469	29.337763220
C	17.602207460	20.656620087	26.316087184
O	18.460393058	20.841405538	25.451183466
C	16.368298457	20.645196521	30.029902879
O	16.540086379	20.825141896	31.238363453
N	16.675687520	21.595714277	26.772209380
C	15.755395463	21.045170427	27.765762903
H	14.705755357	21.147055379	27.418817832
N	15.898456179	21.589215213	29.116787119
C	16.468627009	22.870870784	26.099724057
H	15.390955700	22.972806927	25.851627062
H	17.063718576	22.849214485	25.169748824
C	15.324262832	22.859842104	29.539862042

H	15.243345294	22.831269410	30.640850399
H	14.312308895	22.959075502	29.093360157
N	16.888151106	24.044876160	26.852670498
C	16.068813241	24.682864149	27.881491996
H	15.019960085	24.784530371	27.532166749
N	16.106162903	24.040322679	29.196026672
C	17.970702565	24.833295548	26.459313364
O	18.793770339	24.555455817	25.585168386
C	16.715052638	24.836113019	30.166797719
O	16.838183564	24.557911673	31.362317884
N	17.930850865	26.010270248	27.208204909
C	16.793453879	26.059355858	28.126237584
H	16.159839629	26.944507564	27.908400195
N	17.131028587	26.016140211	29.549304736
C	18.769612759	27.158688852	26.894300501
H	19.249266358	26.958294116	25.919713567
H	18.126085289	28.060583104	26.818254005
C	17.606034605	27.169567465	30.304277190
H	17.048013557	28.068741797	29.969939514
H	17.394188369	26.972385351	31.370143277
N	19.840778540	27.414379416	27.848537677
C	19.656130442	28.164201056	29.092892080
H	19.096874599	29.103169523	28.895078235
N	19.034899655	27.431827506	30.194974719
C	21.185943440	27.293870187	27.488659016
O	21.616742175	26.831988557	26.432417213
C	19.913122610	27.210723079	31.256116146
O	19.627876806	26.698201173	32.339890505
N	21.949172494	27.827505538	28.529568579
C	21.130400050	28.401206383	29.594071969
H	21.385281683	29.472579202	29.737257868
N	21.164185144	27.699751051	30.880116317
C	23.392044428	28.007271407	28.425711171
H	23.649025461	29.038759345	28.742879000
H	23.663300910	27.863685586	27.364750204
C	22.272819030	27.779159021	31.821572419
H	22.659604355	28.819807987	31.841280781
H	21.871956934	27.512078244	32.815592336
N	24.184715000	27.064129505	29.202557845
C	24.476927208	27.206666604	30.626906140
H	24.856248688	28.228176407	30.840268371

N	23.379987140	26.873633209	31.538957560
C	24.868496372	26.000615004	28.614340494
O	24.843742910	25.689332626	27.422712135
C	23.671386104	25.778992553	32.357093294
O	22.959987837	25.337900137	33.261225955
N	25.617396573	25.376541539	29.612546466
C	25.530038670	26.068894136	30.900484860
H	26.529006257	26.447668401	31.202896252
N	24.931320068	25.299271956	31.988678857
C	26.615988177	24.365182592	29.301687739
H	27.600281184	24.688953421	29.701945286
H	26.669260181	24.293154185	28.201021212
C	25.673198439	24.336922870	32.794689608
H	26.698580162	24.730787473	32.956861883
H	25.153940022	24.241797094	33.764856848

Coordinates of the minimized geometry of CB[7]•**3b**.

E: -3200452.2507658 kcal/mol

N	2.014131664	6.912822888	9.032960448
C	1.501483892	8.278776410	8.919484814
H	0.800009888	8.492858705	9.753240041
N	2.508118466	9.337140606	8.825261284
C	1.678122312	6.122169168	7.932588522
O	1.893636180	4.914044252	7.814394265
C	2.460012226	10.012398318	7.604017286
O	3.098056487	11.023025298	7.305515752
N	1.026647063	6.934592054	7.003294536
C	0.817442979	8.294773556	7.501469510
H	-0.268527318	8.524687904	7.534768111
N	1.534551783	9.353972833	6.791913287
C	0.325045940	6.382934118	5.847079784
H	0.322834325	5.283980845	5.957515851
H	-0.718382210	6.762414385	5.849545568
C	1.120172482	9.883997250	5.500257349
H	1.590932375	10.877250548	5.392411570
H	0.014843920	9.989270937	5.486716946
N	0.938503115	6.679808306	4.559475582
C	0.759908749	7.943678305	3.844406185
H	-0.318220375	8.204844668	3.793864409
N	1.528690509	9.082533276	4.350244917

C	1.516725312	5.689186510	3.762115462
O	1.658267743	4.503552827	4.064163120
C	2.469990600	9.542143415	3.426640034
O	3.176497396	10.544534925	3.550997140
N	1.876781361	6.280818542	2.549474203
C	1.406622524	7.661921319	2.436912289
H	0.690596950	7.753653774	1.593028011
N	2.445895381	8.685826488	2.325538896
C	2.373233570	5.504223628	1.421240738
H	1.735424278	5.701605196	0.534039408
H	2.298457199	4.439227117	1.704178435
C	3.126313202	9.011701917	1.074821651
H	3.494247482	10.049576485	1.160499182
H	2.393600085	8.941020586	0.243654239
N	3.764782002	5.764355638	1.063524316
C	4.180603127	6.845445741	0.168116232
H	3.518779794	6.877136995	-0.723172894
N	4.278535453	8.175353715	0.769990021
C	4.767446481	4.809381302	1.247037190
O	4.654095671	3.751228797	1.868447092
C	5.582625241	8.677344831	0.756691866
O	5.925930911	9.816256223	1.075241373
N	5.908820255	5.250216436	0.575718521
C	5.675822723	6.487475055	-0.170333952
H	5.858096084	6.318616702	-1.252704503
N	6.418740155	7.662047940	0.287208183
C	7.060121876	4.380042866	0.352209643
H	6.774668326	3.364176353	0.678258588
H	7.293481200	4.372503355	-0.733309158
C	7.831657337	7.881439438	0.008677798
H	8.021980403	8.962190576	0.133379716
H	8.046919536	7.582093883	-1.038630790
N	8.256883631	4.747282387	1.095723162
C	9.186162685	5.793207956	0.667936719
H	9.456310723	5.650941334	-0.399852366
N	8.748465605	7.170958393	0.895195719
C	8.779427125	3.945974419	2.114074346
O	8.267139277	2.922468048	2.568672970
C	9.550563861	7.839415988	1.822473273
O	9.465062771	9.029257077	2.130643410
N	10.002327793	4.500879338	2.499161560

C	10.402498830	5.625195757	1.652796466
H	11.360734676	5.395069448	1.140767414
N	10.487373405	6.928234195	2.314241099
C	10.897666083	3.840604501	3.439741024
H	10.474386606	2.840962670	3.643268586
H	11.899605234	3.734569243	2.973348130
C	11.630846264	7.352695428	3.115724085
H	11.647195422	8.456945039	3.109542423
H	12.558455582	6.963530043	2.645320069
N	11.049110977	4.519487680	4.722765199
C	12.004799459	5.601292983	4.958934190
H	12.991510747	5.340265700	4.521058121
N	11.590777715	6.930699196	4.508862046
C	10.540960257	3.986939133	5.908839599
O	9.791178079	3.014371027	6.005761195
C	11.460373101	7.839335536	5.561770846
O	11.243709684	9.047687810	5.457471149
N	11.060711672	4.732941395	6.969537052
C	12.027853460	5.738661667	6.526533989
H	13.022563750	5.534913192	6.976187715
N	11.650362122	7.133663037	6.752350113
C	10.928946544	4.297740348	8.355578926
H	10.486186948	3.286076478	8.342367193
H	11.939218828	4.256630482	8.814756717
C	11.740035615	7.794354387	8.047922141
H	11.770584369	8.881792283	7.857405843
H	12.677260246	7.476326152	8.551012172
N	10.068041426	5.135243826	9.179839783
C	10.518574496	6.372631584	9.817249098
H	11.484604730	6.203440119	10.338285101
N	10.616915333	7.543481531	8.945388737
C	8.849765452	4.680727259	9.687936532
O	8.300252855	3.612096479	9.413238774
C	9.705174663	8.542801653	9.288936055
O	9.636646589	9.667386303	8.790598301
N	8.380543000	5.641702095	10.586526061
C	9.333586894	6.733515585	10.788714616
H	9.634270471	6.784082780	11.856525613
N	8.904811206	8.053035564	10.323501042
C	7.222512999	5.411304518	11.442239660
H	7.510451408	5.606874769	12.496467387

H	6.935418542	4.351297566	11.324902239
C	7.988164156	8.911735018	11.062732014
H	8.165886837	9.947931410	10.724560742
H	8.212567300	8.829117643	12.147075476
N	6.047707762	6.213076581	11.117061582
C	5.844868075	7.586219022	11.580666881
H	6.063948448	7.658089654	12.666966166
N	6.574728389	8.623455559	10.851078296
C	4.880903930	5.646190165	10.601905765
O	4.734194773	4.474697025	10.249902062
C	5.726155005	9.510421132	10.186767659
O	6.068246273	10.531544512	9.586245052
N	3.896982462	6.637127547	10.586414880
C	4.340195424	7.878529595	11.221145727
H	3.707346763	8.102319878	12.105791776
N	4.417383112	9.051602276	10.349487893
C	2.504334477	6.337941523	10.281180318
H	2.419207892	5.240352863	10.193269257
H	1.864977974	6.697325333	11.114821441
C	3.257466138	9.850062292	9.966188369
H	2.576522176	9.932993781	10.839217044
H	3.627592112	10.852011771	9.685096697
N	5.397378361	3.060631659	6.069978285
C	5.749391318	4.631265043	5.902711314
C	4.611733136	2.544694231	4.875043711
H	5.136518200	2.794294712	3.940222873
H	3.607775859	2.996123449	4.865376112
H	4.527888289	1.449817917	4.978855818
C	6.662996973	2.227018674	6.188699775
H	6.360832120	1.195820135	6.437310944
H	7.304872978	2.629295595	6.987500219
H	7.204728139	2.236212881	5.231527089
C	4.560999029	2.814794171	7.317130305
H	3.679969416	3.476520791	7.319763341
H	5.166408599	2.999037039	8.216833406
H	4.235811515	1.761024539	7.295039251
C	6.270468218	5.189583069	7.247348922
H	7.167276577	4.637659519	7.578338072
H	5.510547375	5.077850820	8.037981599
C	4.482125869	5.408674820	5.477430474
H	3.664352329	5.264825902	6.205218943

H	4.119874059	5.050219023	4.499948570
C	6.837404817	4.823060896	4.818888433
H	6.498642889	4.423094857	3.846836559
H	7.764429179	4.291075400	5.091998437
C	6.612337711	6.691554596	7.098259560
H	6.987139145	7.059377771	8.075672220
C	4.811981761	6.916228145	5.355265592
H	3.882179584	7.450324744	5.075645191
C	7.159528859	6.332078544	4.669820829
H	7.936137637	6.440970973	3.887178573
N	7.097027046	10.776296730	5.329748113
C	7.866690893	11.272999182	6.544416416
H	8.871616093	10.826704604	6.557905071
H	7.325506687	11.009105154	7.467169648
H	7.945795094	12.370070156	6.461396673
C	5.828575392	11.607379354	5.213708999
H	6.130004100	12.642262669	4.979690655
H	5.277417235	11.586358575	6.166006019
H	5.188342504	11.212862786	4.409278913
C	7.943972723	11.048139596	4.097299952
H	7.344236572	10.876619176	3.190539148
H	8.824536656	10.388127258	4.091093779
H	8.265686299	12.102382932	4.138534341
C	6.241558157	8.647787759	4.112061444
H	7.010731546	8.752505401	3.328821767
H	5.345292404	9.197961374	3.774923815
C	8.027705285	8.419954511	5.868392574
H	8.427789021	8.784131132	6.829539592
H	8.821337384	8.551395676	5.112048594
C	5.658563359	9.000983939	6.535032385
H	4.733317067	9.520976035	6.237758781
H	5.971006636	9.421770493	7.506352030
C	5.897039492	7.144333501	4.266104238
H	5.517241502	6.778707035	3.292037688
C	7.695809925	6.913783540	6.007490039
H	8.623531471	6.382496618	6.301933713
C	5.345596721	7.494306773	6.694550532
H	4.575019119	7.383261799	7.484385916
C	6.754800877	9.200557157	5.463250282

Coordinates of the minimized geometry of CB[7]•**3c**.

N	2.00900	6.90900	9.03700
C	1.50900	8.27700	8.91600
H	0.80300	8.49400	9.74800
N	2.50800	9.34100	8.82600
C	1.62800	6.10700	7.95700
O	1.75900	4.88500	7.88000
C	2.43200	10.04000	7.61800
O	3.01200	11.09200	7.35000
N	1.02100	6.93100	7.00500
C	0.82500	8.29400	7.49700
H	-0.26100	8.52700	7.53500
N	1.53600	9.35700	6.79000
C	0.32200	6.38400	5.84800
H	0.32100	5.28500	5.95800
H	-0.72300	6.76300	5.84700
C	1.11400	9.88700	5.50000
H	1.58400	10.88200	5.39200
H	0.00700	9.99200	5.49200
N	0.93900	6.67900	4.56200
C	0.76600	7.94300	3.84800
H	-0.31500	8.19900	3.79200
N	1.52100	9.09300	4.34700
C	1.48600	5.67900	3.75100
O	1.56300	4.48300	4.02800
C	2.42600	9.58200	3.40000
O	3.05800	10.63500	3.47900
N	1.87700	6.27800	2.55000
C	1.41400	7.66000	2.44100
H	0.69400	7.75000	1.59800
N	2.44300	8.69200	2.32300
C	2.36900	5.50400	1.41800
H	1.72700	5.70200	0.53300
H	2.29700	4.43800	1.70100
C	3.12300	9.01300	1.07200
H	3.49000	10.05100	1.15900
H	2.39200	8.94100	0.23800
N	3.76000	5.75900	1.05800
C	4.18100	6.84700	0.17600
H	3.52300	6.88100	-0.72000
N	4.27800	8.17900	0.77100
C	4.74700	4.77800	1.19700

O	4.60500	3.68000	1.73200
C	5.57800	8.69100	0.72800
O	5.91100	9.84700	0.98500
N	5.90600	5.24500	0.57000
C	5.67700	6.48900	-0.16300
H	5.85600	6.32400	-1.24800
N	6.42000	7.66500	0.28800
C	7.05900	4.37900	0.34800
H	6.77200	3.36300	0.67500
H	7.29700	4.37100	-0.73700
C	7.83200	7.88200	0.00600
H	8.02400	8.96200	0.13200
H	8.04400	7.58300	-1.04300
N	8.25300	4.74500	1.09700
C	9.17900	5.79400	0.67500
H	9.45300	5.64800	-0.39300
N	8.75100	7.17500	0.89100
C	8.79100	3.92500	2.09500
O	8.31000	2.87000	2.50600
C	9.58800	7.85700	1.78000
O	9.56600	9.06300	2.01500
N	10.00100	4.49700	2.50100
C	10.39700	5.62500	1.66000
H	11.35300	5.39200	1.14300
N	10.49200	6.93100	2.31100
C	10.89900	3.84000	3.44000
H	10.47600	2.84000	3.64500
H	11.90100	3.73400	2.97100
C	11.63500	7.35200	3.11400
H	11.64900	8.45700	3.10600
H	12.56500	6.96200	2.64600
N	11.04900	4.51600	4.72400
C	11.99500	5.60400	4.95900
H	12.98500	5.34300	4.52300
N	11.59100	6.93400	4.50800
C	10.58400	3.94900	5.91400
O	9.91400	2.92300	6.01500
C	11.49100	7.85000	5.56100
O	11.34000	9.06600	5.45500
N	11.06600	4.72500	6.97200
C	12.02000	5.74100	6.52700

H	13.01900	5.54000	6.97200
N	11.64900	7.13600	6.75300
C	10.93300	4.29600	8.35900
H	10.49100	3.28400	8.34500
H	11.94300	4.25700	8.82300
C	11.74100	7.79400	8.05000
H	11.77100	8.88200	7.85900
H	12.68000	7.47500	8.55200
N	10.06700	5.13200	9.17900
C	10.51200	6.37300	9.81000
H	11.47700	6.20300	10.33500
N	10.61800	7.54800	8.94700
C	8.86600	4.65800	9.71700
O	8.35600	3.56000	9.50100
C	9.73800	8.56600	9.32400
O	9.73000	9.71700	8.89100
N	8.37900	5.63800	10.58800
C	9.32700	6.73400	10.78200
H	9.63200	6.78200	11.85000
N	8.90500	8.05800	10.32700
C	7.22200	5.41100	11.44500
H	7.51100	5.60800	12.50000
H	6.93500	4.35100	11.32800
C	7.98800	8.91300	11.06900
H	8.16700	9.94900	10.73100
H	8.21200	8.82900	12.15400
N	6.04700	6.20900	11.11800
C	5.84600	7.58500	11.57200
H	6.06100	7.65700	12.66000
N	6.57600	8.62800	10.85300
C	4.86600	5.62900	10.64500
O	4.69800	4.44200	10.37400
C	5.72200	9.54100	10.22600
O	6.05400	10.60300	9.70100
N	3.89400	6.63300	10.58800
C	4.34100	7.87700	11.21200
H	3.71100	8.10100	12.10000
N	4.41700	9.05500	10.34900
C	2.50000	6.33800	10.28600
H	2.41400	5.24000	10.19700
H	1.86100	6.69800	11.12200

C	3.25500	9.85100	9.96900
H	2.57300	9.93400	10.84300
H	3.62600	10.85300	9.68800
C	5.39300	3.02200	6.07300
C	5.74000	4.58100	5.90700
C	4.59200	2.49000	4.85100
H	5.09600	2.70900	3.89100
H	3.58000	2.93100	4.79100
H	4.47700	1.38700	4.93200
C	6.68800	2.16900	6.19600
H	6.42000	1.11800	6.43700
H	7.35800	2.53800	6.99500
H	7.27200	2.16300	5.25700
C	4.53900	2.76800	7.34800
H	3.63900	3.41000	7.39000
H	5.11000	2.95100	8.27700
H	4.19900	1.70900	7.36300
C	6.27100	5.18900	7.24000
H	7.16800	4.63300	7.57300
H	5.51400	5.06900	8.03600
C	4.48800	5.40700	5.47900
H	3.66500	5.25800	6.20300
H	4.12000	5.04200	4.50300
C	6.83200	4.82500	4.82000
H	6.49400	4.42000	3.84800
H	7.75900	4.28500	5.08500
C	6.61200	6.68800	7.09500
H	6.99000	7.06800	8.07000
C	4.81300	6.91200	5.35400
H	3.88700	7.45700	5.07300
C	7.15700	6.33000	4.66800
H	7.93500	6.45000	3.88500
C	7.10800	10.81300	5.32500
C	7.89700	11.32200	6.56700
H	8.91200	10.88700	6.62300
H	7.38500	11.08100	7.51800
H	8.00300	12.42700	6.51200
C	5.81400	11.66600	5.20600
H	6.08200	12.72200	4.98200
H	5.22100	11.66100	6.14000
H	5.14600	11.30900	4.40100

C	7.97700	11.09300	4.06700
H	7.41900	10.91200	3.12900
H	8.88300	10.45900	4.03300
H	8.30600	12.15500	4.06800
C	6.24100	8.64800	4.11800
H	7.00700	8.76100	3.32900
H	5.34700	9.20300	3.77600
C	8.02300	8.42000	5.86300
H	8.43200	8.79000	6.82000
H	8.81800	8.55600	5.10600
C	5.66400	9.00000	6.53100
H	4.73900	9.52800	6.23900
H	5.97500	9.42500	7.50300
C	5.89800	7.14700	4.26500
H	5.51600	6.77100	3.29300
C	7.69500	6.91700	6.00400
H	8.62000	6.37400	6.29700
C	5.34800	7.49700	6.69200
H	4.57500	7.37400	7.48100
C	6.76600	9.25000	5.45800

Coordinates of the minimized geometry of CB[7]•9.

E: -3100400.05066236 kcal/mol

N	24.197490481	6.841380275	12.366777466
C	24.194828640	8.164794266	11.746011328
H	23.151242647	8.502243330	11.570755480
N	24.948682568	9.199137888	12.456910380
C	24.927113318	5.903071557	11.634579837
O	25.066986745	4.710881567	11.915296820
C	26.032983288	9.679871445	11.718475567
O	26.763872401	10.621097046	12.027694478
N	25.424449118	6.551839707	10.501890481
C	25.022618831	7.955192535	10.426141456
H	24.439798048	8.136839138	9.498354238
N	26.104335814	8.931505213	10.540294667
C	26.022704560	5.838594532	9.384225133
H	25.832308623	4.761991113	9.539455252
H	25.536890192	6.172345946	8.443843507
C	27.000608033	9.277454503	9.444794239
H	27.399294729	10.286025565	9.654016662

H	26.421298772	9.291215265	8.498456695
N	27.462770819	6.006997576	9.254623683
C	28.116105862	7.117662432	8.560722165
H	27.669573488	7.257380355	7.554002050
N	28.147970408	8.392193765	9.281328086
C	28.348505095	4.989912269	9.602361644
O	28.051868770	3.920061071	10.137825301
C	29.440693196	8.782947916	9.629536282
O	29.758000317	9.845075393	10.170641939
N	29.623410748	5.384009928	9.205072784
C	29.632866170	6.681117312	8.527092782
H	30.044506811	6.574900379	7.501540474
N	30.312126198	7.769109670	9.234046237
C	30.759099387	4.476657126	9.283540559
H	31.314813695	4.515621593	8.323738898
H	30.355247537	3.460667177	9.439428656
C	31.760072674	7.905067754	9.344487437
H	32.221745643	7.614792259	8.378130696
H	31.968627078	8.969324262	9.553891672
N	31.682835233	4.749462482	10.373422168
C	32.766731092	5.725250151	10.272700691
H	33.328340295	5.577470103	9.326028101
N	32.374210387	7.125989539	10.411394644
C	31.795795135	3.922901974	11.493949828
O	31.052688333	2.984894515	11.789120688
C	32.859392073	7.708821249	11.584986790
O	32.743719360	8.889948959	11.912047592
N	32.937099473	4.321168659	12.192605774
C	33.619061570	5.450944688	11.564920942
H	34.677987464	5.189528054	11.355342410
N	33.545296473	6.718912277	12.293793712
C	33.540077429	3.497033710	13.230405206
H	34.609984723	3.336774439	12.976953401
H	33.010575817	2.527962771	13.233543264
C	34.403098367	7.036289185	13.426049601
H	34.387185759	8.133897590	13.547550717
H	35.438922892	6.702023470	13.198515415
N	33.451177692	4.036941748	14.578035944
C	34.336487637	5.079786922	15.087405492
H	35.389407930	4.857220589	14.812038389
N	33.994645961	6.450706041	14.697563723

C	32.714977154	3.410973498	15.584308983
O	31.962538231	2.446241938	15.441824189
C	33.632515299	7.240898992	15.791695224
O	33.377867746	8.446757371	15.770274978
N	33.028806080	4.039616992	16.791509180
C	34.070197670	5.058476887	16.636971020
H	34.962002551	4.786920971	17.240783496
N	33.665703471	6.429536765	16.926862756
C	32.631805167	3.479691613	18.077487456
H	33.536930474	3.339507014	18.705604226
H	32.164305035	2.500010683	17.873325542
C	33.557912883	6.958998807	18.276353701
H	34.395421511	6.556935377	18.884641477
H	33.640938888	8.058118241	18.208252366
N	31.663096437	4.271305808	18.825260753
C	32.019948546	5.416831930	19.662427081
H	32.870043600	5.154228343	20.326833581
N	32.301591748	6.666066161	18.951962763
C	30.338929288	3.869284081	18.994976937
O	29.800392877	2.889945478	18.474243231
C	31.378309966	7.669810211	19.238369130
O	31.417167359	8.833597832	18.835544526
N	29.737343351	4.757508970	19.890936337
C	30.685283390	5.733427650	20.436829415
H	30.767979385	5.611817588	21.537359717
N	30.423947664	7.129811726	20.100756687
C	28.402355732	4.531429480	20.434890808
H	28.447337901	4.606882868	21.541437107
H	28.100142169	3.509743766	20.143180027
C	29.397971381	7.946796145	20.730811690
H	29.345894251	7.690008743	21.808542571
H	29.701354900	9.001874812	20.611099777
N	27.375203994	5.441980085	19.940098579
C	27.116489640	6.767922003	20.509664689
H	27.021577844	6.698047942	21.613693517
N	28.071219113	7.811771719	20.149406094
C	26.358696515	5.021319697	19.077907750
O	26.270948362	3.910933390	18.549434351
C	27.524372494	8.784386918	19.311966575
O	28.100279414	9.790669262	18.895113863
N	25.448296223	6.069970763	18.953651143

C	25.792075456	7.221812655	19.787377925
H	24.958994602	7.450621544	20.484956207
N	26.197661854	8.433022697	19.070748430
C	24.179438499	5.926072593	18.251195355
H	23.364887500	6.292415840	18.911038137
H	24.039027671	4.849525047	18.047848562
C	25.270932391	9.355893901	18.430775438
H	25.786106556	10.329442611	18.350831283
H	24.368861458	9.460425946	19.069908846
N	24.098545731	6.617115210	16.970529550
C	23.764639260	8.036503763	16.833359473
H	22.887087896	8.284749749	17.467446698
N	24.852415916	8.973736343	17.092052219
C	23.996089011	5.925371265	15.761644218
O	24.111353051	4.708720269	15.608792896
C	25.270890283	9.654305683	15.947438863
O	26.127034841	10.539798044	15.903219149
N	23.683242311	6.854426095	14.768751274
C	23.500963176	8.205030651	15.292479422
H	22.481632459	8.574788840	15.051668148
N	24.503493399	9.189214301	14.876178319
C	23.280859373	6.453768690	13.429897808
H	22.281379892	6.886354919	13.209151804
H	23.216109672	5.351409496	13.426910081
C	24.425346273	9.912657920	13.612676423
H	25.023176350	10.834759357	13.722321754
H	23.362673917	10.178339551	13.421667627
C	27.671500801	2.498135301	12.959466537
H	26.906873524	3.151405300	12.509407851
H	27.371298829	1.441914559	12.864951564
H	28.651316562	2.658004751	12.481246263
C	26.414897081	2.549258665	15.085030532
H	26.471939780	2.737596865	16.168650493
H	26.135867576	1.500248664	14.889404020
H	25.690498576	3.247089165	14.634912347
C	28.831071124	1.862143412	15.042672961
H	29.800961147	2.080442554	14.566914873
H	28.511583814	0.825760806	14.842441890
H	28.912809598	2.036774266	16.126761936
N	27.781223505	2.799846175	14.447333950
C	28.192239962	4.231548558	14.717979025

C	28.412167539	5.125073311	13.680857452
H	28.295305246	4.840110030	12.630940945
C	28.806218691	6.466672011	13.978090435
C	29.047186072	7.425250245	12.948763840
H	28.917000079	7.126804764	11.901386051
C	29.438217979	8.720462980	13.251713573
H	29.614152426	9.420945615	12.427506136
C	28.344749330	4.625409358	16.079318279
H	28.166535628	3.922330312	16.898680342
C	28.727356507	5.922298437	16.383237177
H	28.846434522	6.222556448	17.432630492
C	28.971100478	6.875835716	15.350706951
C	29.372039105	8.213876487	15.648092625
H	29.487964176	8.494434255	16.698915773
C	29.600439849	9.107870977	14.614111201
N	30.033369150	10.530492488	14.895915078
C	30.160704954	10.814920960	16.385001215
H	29.185769700	10.661416979	16.875403579
H	30.476894443	11.865413278	16.488637941
H	30.917986925	10.146600023	16.825519576
C	28.991889276	11.490430190	14.319799809
H	28.893142994	11.322559620	13.237016806
H	29.332170235	12.519694100	14.523381163
H	28.027702079	11.279742686	14.812933849
C	31.400110320	10.766275960	14.251716245
H	32.114379247	10.057736707	14.704464595
H	31.691892493	11.811358501	14.449683053
H	31.335822378	10.579908781	13.169332848

Plot of ΔG_{exptl} versus ΔG_{calcd}

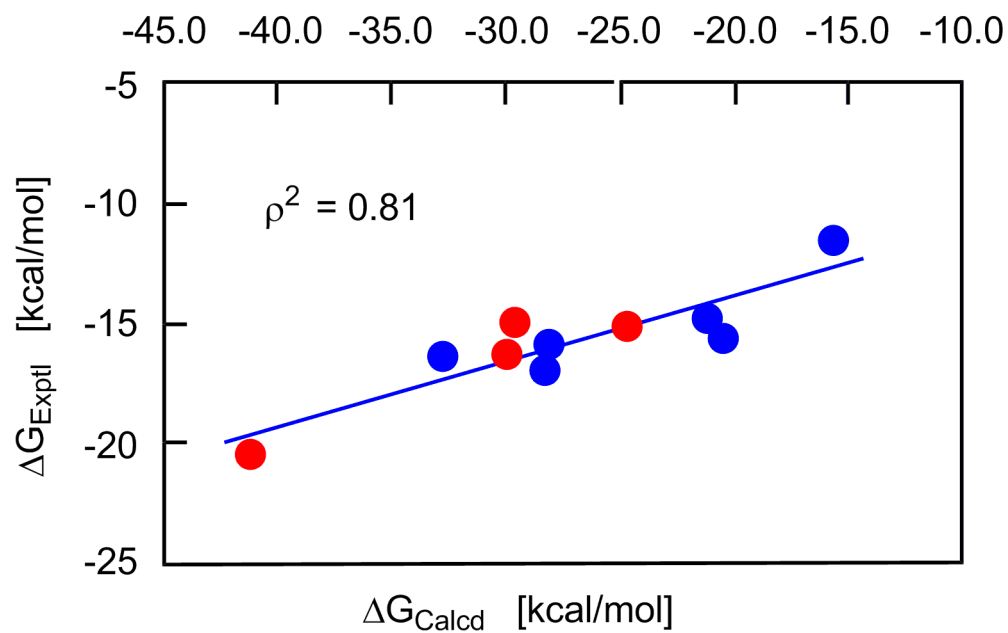


Figure S20. Least squares linear plot of ΔG_{Exptl} versus ΔG_{calcd} , $r^2 = 0.81$, calculated for a set of ten CB[7]•guest complexes. The red circles are the four $-di(^+NMe_3)$ complexes in Tables 2-3.

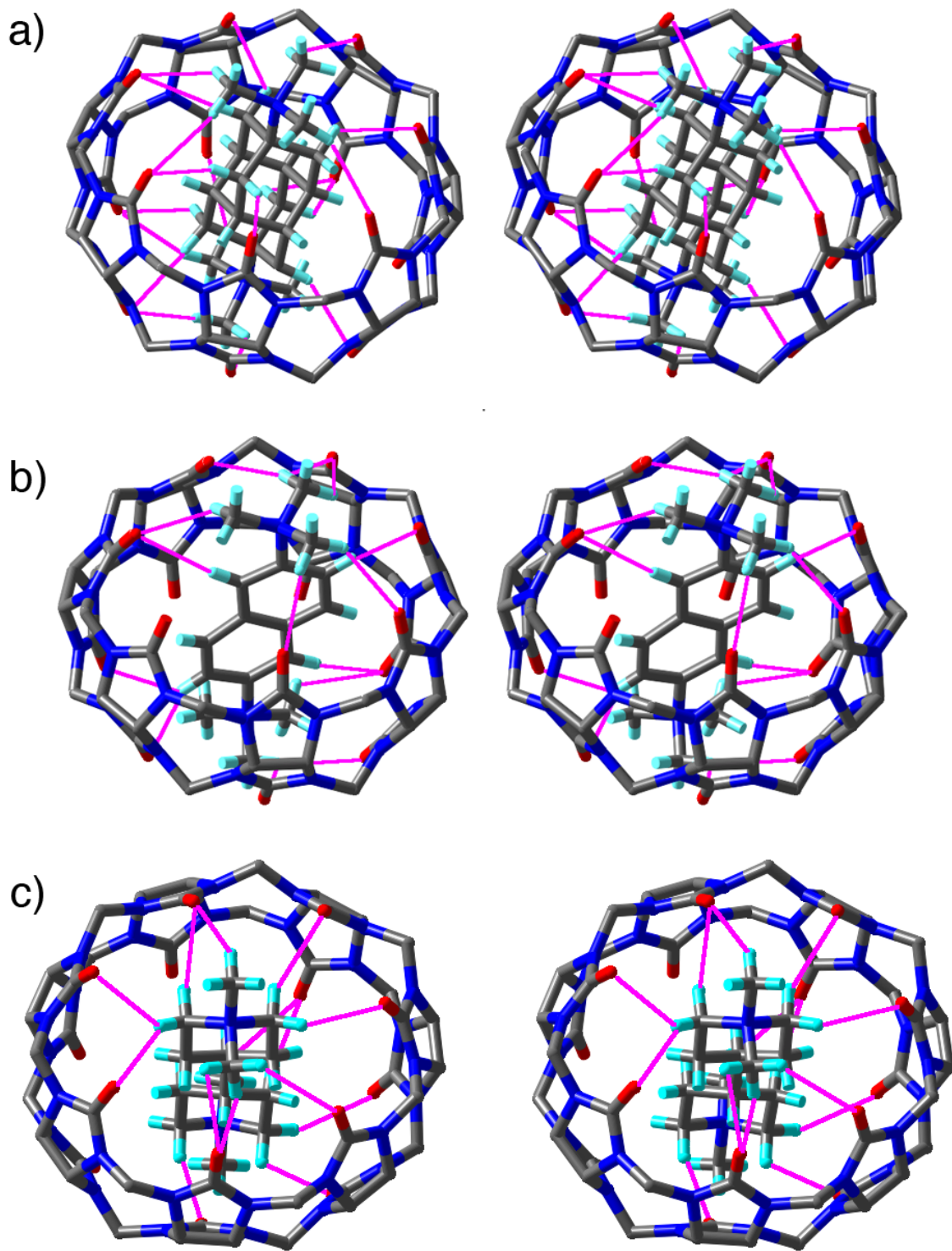


Figure S21. Stereoviews rendered from the x-crystal structures of: a) CB[7]•**3b**, b) CB[7]•**9**, and c) CB[7]•**14** to illustrate the presence of numerous C-H...O=C close contacts ($\leq 2.70\text{\AA}$). Color code: C, grey; H, light blue; N, blue; O, red; C-H...O=C close contacts, magenta.