

Supramolecular β - Cyclodextrin – Aniline system: A new class of amine on solid support for carbon dioxide capture with high amine efficiency

Deepthi L. Sivadas,^{a, b} K.P. Vijayalakshmi,^b R. Rajeev,^b K. Prabhakaran^a and K. N. Ninan^a

1. ^1H NMR spectrum of β -cyclodextrin – aniline complex

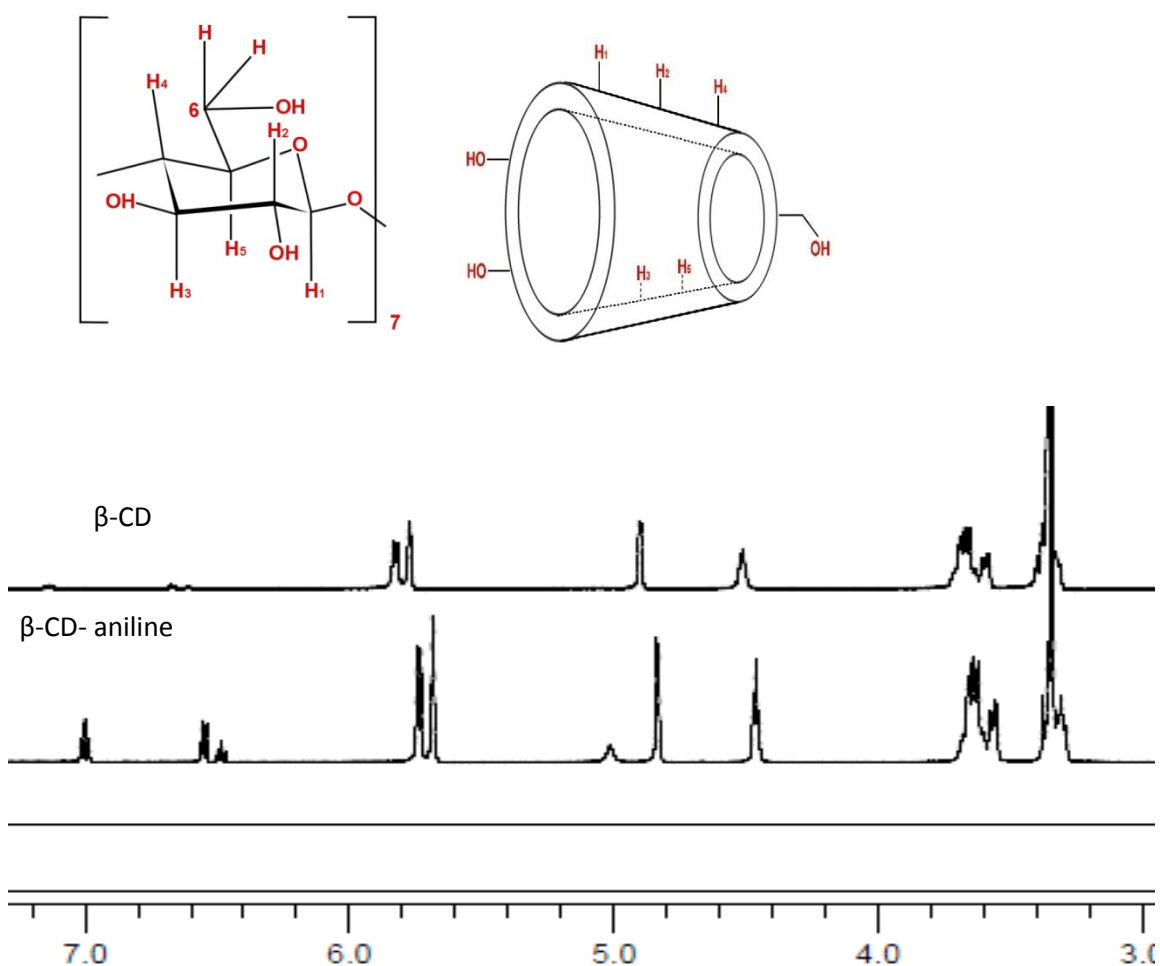


Fig. 1: ^1H NMR spectrum of β - cyclodextrin – aniline inclusion complex in DMSO-d_6

Table 1: Chemical shift values of β - cyclodextrin protons after complex formation

	H1	H2	H3	H4	H5	H6
β -CD	4.89	3.38	3.82	3.45	3.74	3.79
β -CD-aniline complex	4.83	3.31	3.67	3.37	3.57	3.62
$\Delta\delta$	0.06	0.07	0.15	0.08	0.17	0.17

Elemental analysis

Table 2: Elemental analysis of β -CD and 1:1 β -CD - aniline complex

Compound	Carbon, %	Hydrogen, %	Nitrogen, %
β -cyclodextrin	44.45	6.22	-
β -cyclodextrin-aniline complex	46.8	7.1	1.1

Molecular modeling

Full citation for Gaussian09

Gaussian 09, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Optimized structure of CD...Aniline...(2H₂O) complex at PM6 level (X, Y, Z coordinates are given in Å).

SCF energy = -2.67123111292 A.U.

Number of imaginary frequencies = 0

Atom	X	Y	Z
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C	-4.486903000	-3.900910000	1.472844000
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C	-6.765548000	0.585069000	-0.949748000
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H	-4.196874000	-1.228124000	1.593087000
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Optimized structure of CD...C₆H₅NH₃⁺...(HCO₃⁻)...H₂O complex at PM6 level (X, Y, Z coordinates are given in Å).

SCF energy = -2.82940017437 A.U.

Number of imaginary frequencies = 0

Atom	X	Y	Z
C	0.441736000	-5.281071000	-0.728350000
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H	-6.898772000	-1.431909000	0.063791000
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H	-5.959957000	-0.579828000	2.643019000
H	-5.514950000	-2.160225000	3.430854000
H	0.165140000	-3.162614000	-3.171402000
H	-3.415315000	-4.133050000	-2.670341000
H	-0.356772000	-5.813016000	3.156253000
H	5.699676000	-4.163190000	-2.577479000
H	2.481616000	-4.807189000	-2.693792000
H	0.918386000	-5.513320000	1.866491000

H	3.393478000	0.751274000	-3.200497000
H	4.600291000	-2.096849000	-2.493588000
H	8.493522000	-1.062829000	0.007469000
H	1.238317000	4.352141000	-2.068515000
H	4.675854000	4.441303000	-3.116493000
H	2.491941000	3.754482000	3.697806000
H	-2.968428000	6.547270000	-1.993317000
H	0.286669000	6.355413000	-1.884489000
H	1.545905000	4.951388000	2.456720000
H	-4.028470000	-0.018354000	-2.033436000
H	-3.852535000	4.284105000	-2.372454000
H	-6.853944000	4.353760000	1.435239000
H	-5.554681000	-4.154462000	-3.031519000
H	-5.913785000	-1.006479000	-2.766441000
H	-7.408353000	-3.008779000	2.326099000
C	1.054018000	-0.447827000	3.560949000
C	1.768396000	0.367694000	2.676830000
C	0.340263000	-1.552252000	3.082083000
H	2.331998000	1.234868000	3.057422000
H	-0.222265000	-2.186290000	3.771335000
C	1.774874000	0.087521000	1.308442000
C	0.340491000	-1.848712000	1.716942000
H	2.321773000	0.734866000	0.609548000
H	-0.212745000	-2.722180000	1.343998000
C	1.061591000	-1.025486000	0.845195000
H	1.054921000	-0.220562000	4.628287000
N	1.048091000	-1.315324000	-0.608956000
H	0.896614000	-2.333451000	-0.818292000
H	1.943463000	-1.012096000	-1.062272000
H	2.482090000	1.844577000	-1.686563000
O	1.778707000	1.123021000	-1.583944000
C	0.453145000	1.581963000	-1.829636000
O	0.309049000	2.761613000	-2.116303000
O	-0.365317000	0.633088000	-1.694677000
H	0.269982000	-0.704037000	-1.100668000
O	-2.403896000	-0.629771000	-1.754214000
H	-2.114903000	-0.079462000	-1.002600000
H	-1.936245000	-0.229269000	-2.519426000