Supporting Information

A Quantitative Study of Intrinsic Non-covalent Interactions within Complexes of α-Cyclodextrin and Benzoate Derivatives**

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1. Threshold CID Measurements

The determination of absolute gas-phase reaction barriers requires the reactant ions to be prepared with well-defined, narrow distributions of their kinetic and internal energies prior to collision.[21] On the customized Finnigan MAT TSQ-700 mass spectrometer, this is accomplished by thermalizing the electrosprayed ions with 10 mTorr argon in a gas cell mounted on a radiofrequency 24-pole ion guide. Retardation measurements, in which the parent ion intensity is recorded as a function of the *dc* bias potential applied to the collision octapole in the absence of collision gas, afford well-defined near-Gaussian distributions of the ions' kinetic (and presumably internal) energies (Figures S1–S3) as required for subsequent deconvolution of the cross-section curves. For the CID threshold measurements, the parent ion was mass-selected in the first quadrupole and allowed to react with xenon in the octapole collision cell. Intensities of the reactant and product ions were recorded as a function of the collision offset voltage (Figures S4–S6). These intensities were converted to reactive collision cross sections according to Ervin et al.,[22] extrapolated to zero collision-gas pressure to impose single-collision conditions, and fitted with L-CID (Figures S7-S9).[6a,b] Three independent data sets were acquired on different days; the Figures are derived from data set 3. For each data set, at least 15 acceptable fits were selected to determine the confidence intervals of the fitting parameters, and the final values of the parameters were obtained as averages over the data sets. For an accurate treatment of the kinetic shift, one needs to distinguish between so-called "loose" and "tight" transition states.[6a] A loose transition–state (TS) model is appropriate for reactions in which the dissociation into products is rate limiting (*i.e.* a reverse activation barrier is absent); otherwise, a tight TS model should be used. Both loose and tight transition-state models were considered (Tables S1–S3); DFT calculations (see below) indicate that the rate-limiting transition state is loose for the fragmentation of $[\alpha\text{-CD}\cdot\text{RBA}]^-$ into $[\alpha\text{-CD}]^-$ and RBA. Using these arguments, we obtained benchmark values for the threshold dissociation energy E_0 of 40.8(5), 41.1(5), and 41.8(5) kcal mol^{-1} for the complexes **1**, **2**, and **3**, respectively.

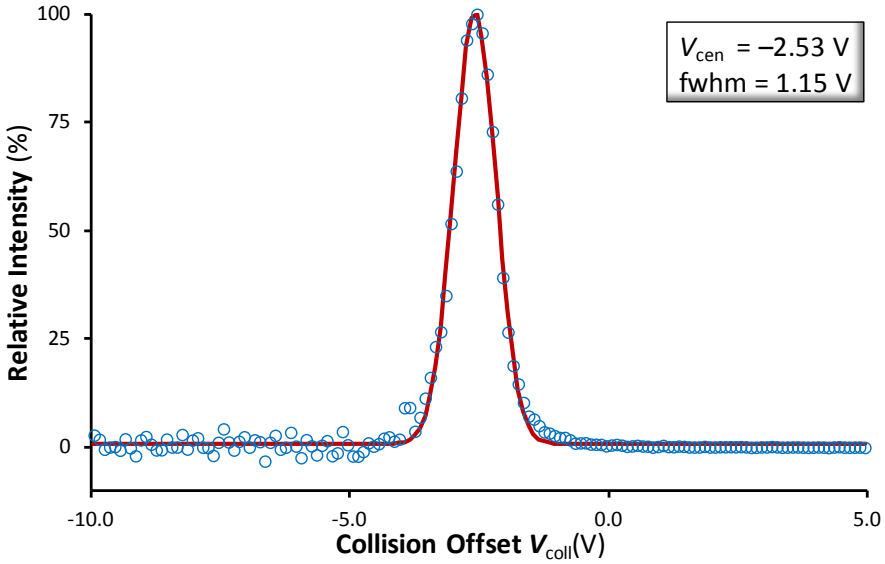


Figure S1. Distribution of uncorrected ion kinetic energies in the laboratory frame for [α-CD·3-MeBA]$^-$; the Gaussian fit (red line) has a full width at half-maximum of 1.15eV.

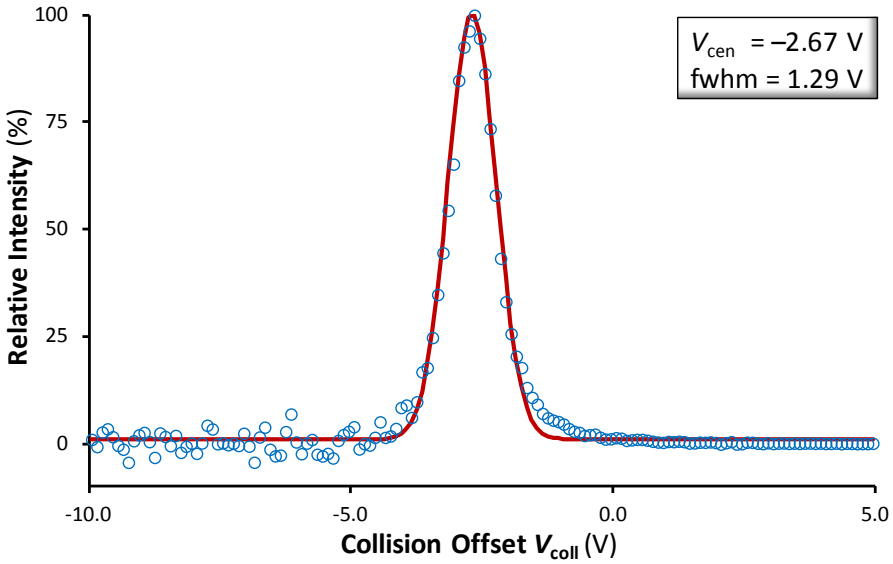


Figure S2. Distribution of uncorrected ion kinetic energies in the laboratory frame for [α-CD·BA]$^-$; the Gaussian fit (red line) has a full width at half-maximum of 1.29eV.

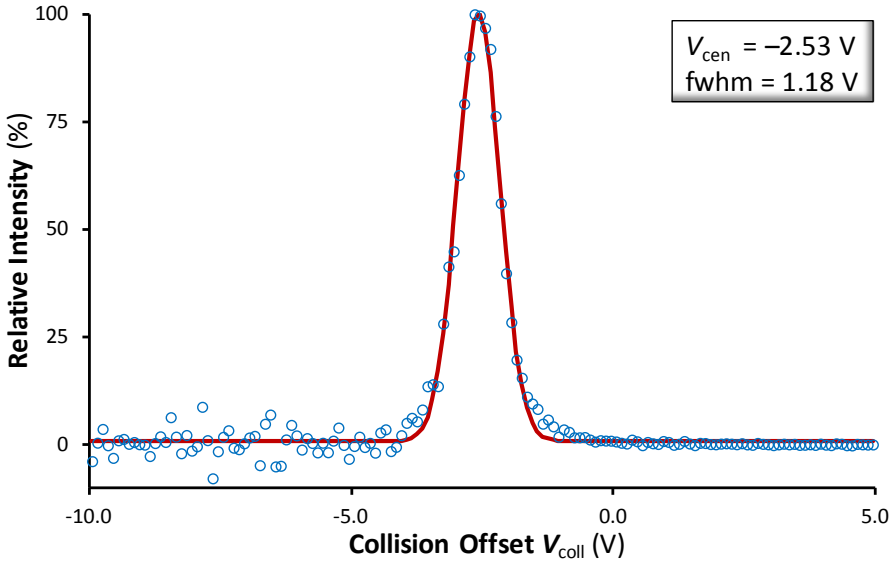


Figure S3. Distribution of uncorrected ion kinetic energies in the laboratory frame for [α-CD·3-OHBA]⁻; the Gaussian fit (red line) has a full width at half-maximum of 1.18eV.

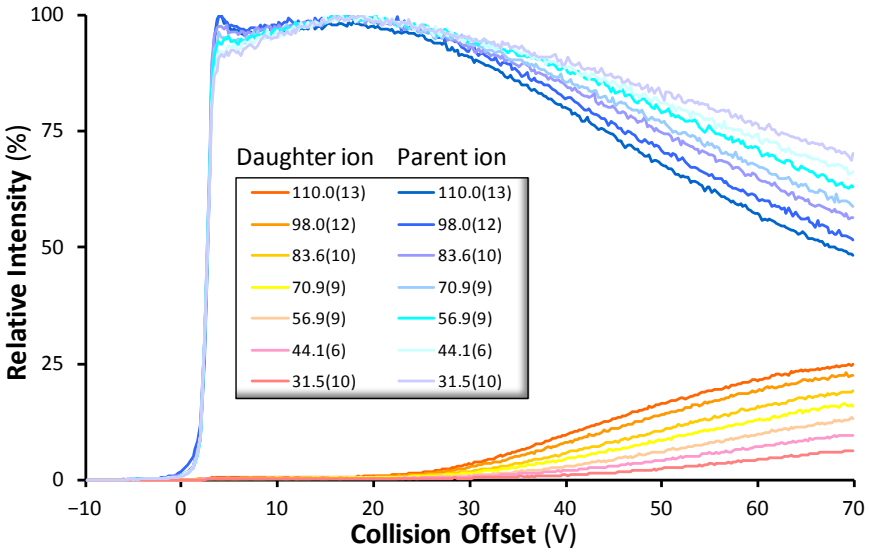


Figure S4. Ion intensity curves for CID of [α-CD·3-MeBA]⁻ with xenon as collision gas at different pressures (μTorr).

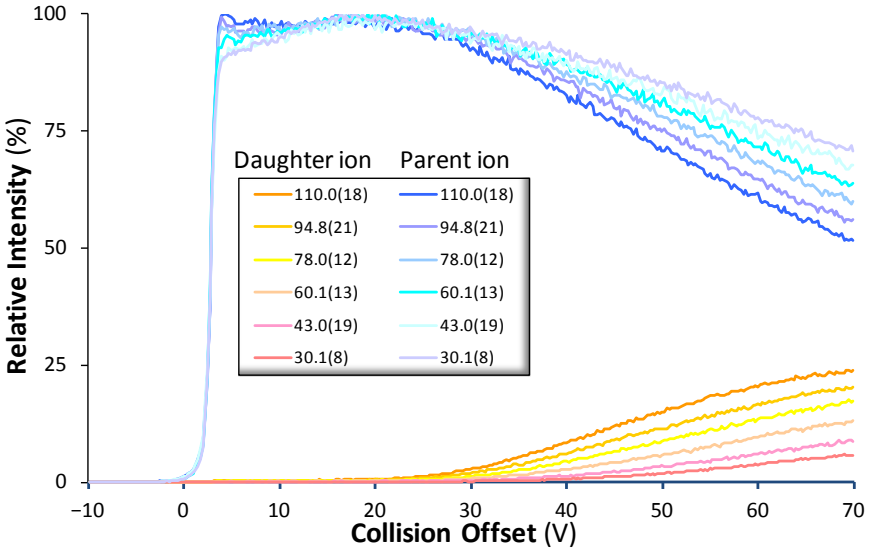


Figure S5. Ion intensity curves for CID of [α-CD·BA]$^-$ with xenon as collision gas at different pressures (μTorr).

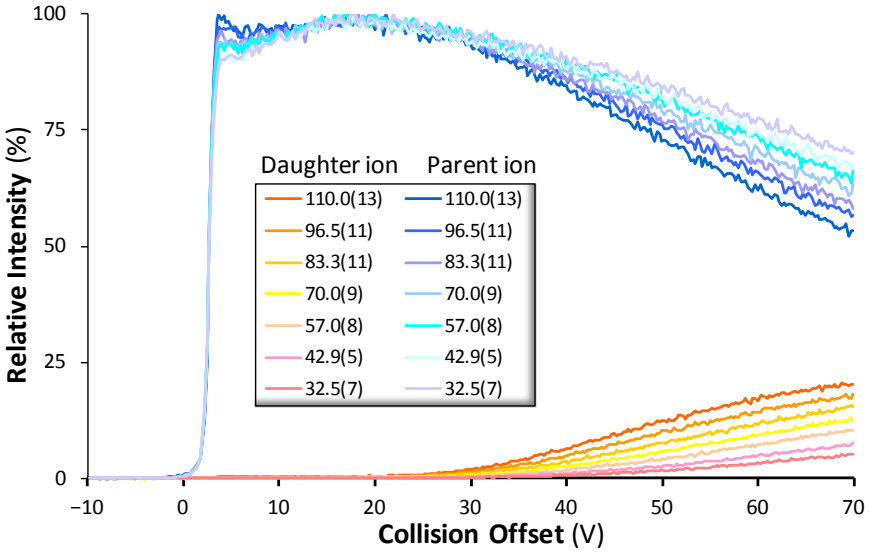


Figure S6. Ion intensity curves for CID of [α-CD·3-OHBA]$^-$ with xenon as collision gas at different pressures (μTorr).

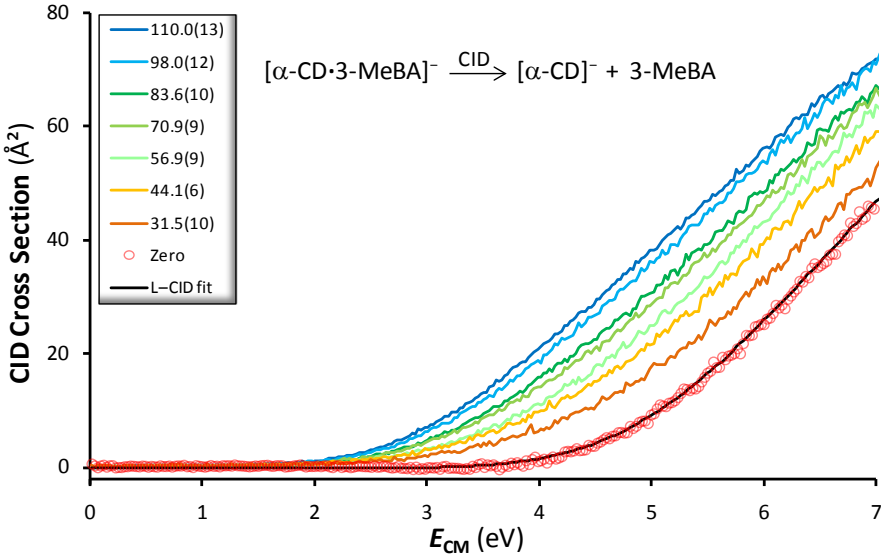


Figure S7. Threshold reactive collision cross-section curves for the dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{3-MeBA}]^-$ at various collision gas pressures, extrapolation to zero pressure, and fitted curve from L-CID assuming no reverse barrier.

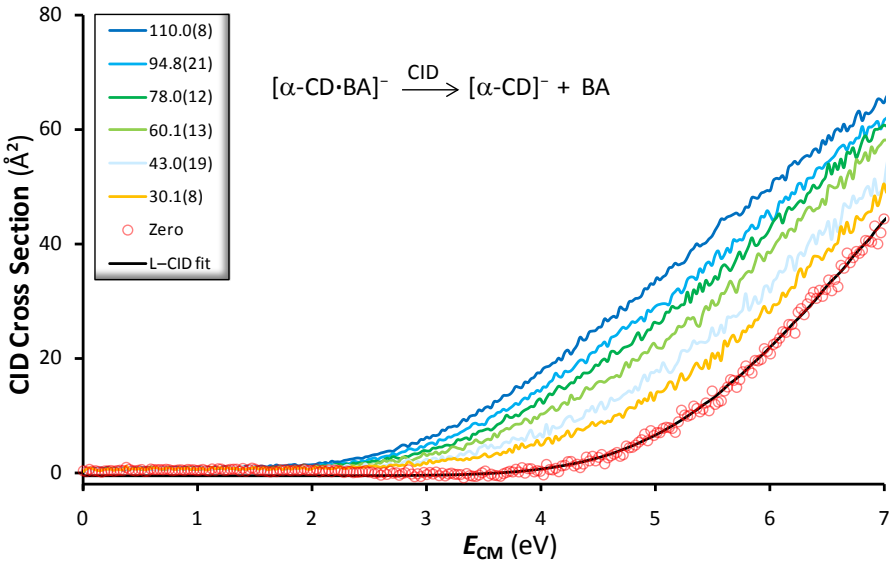


Figure S8. Threshold reactive collision cross-section curves for the dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{BA}]^-$ at various collision gas pressures, extrapolation to zero pressure, and fitted curve from L-CID assuming no reverse barrier.

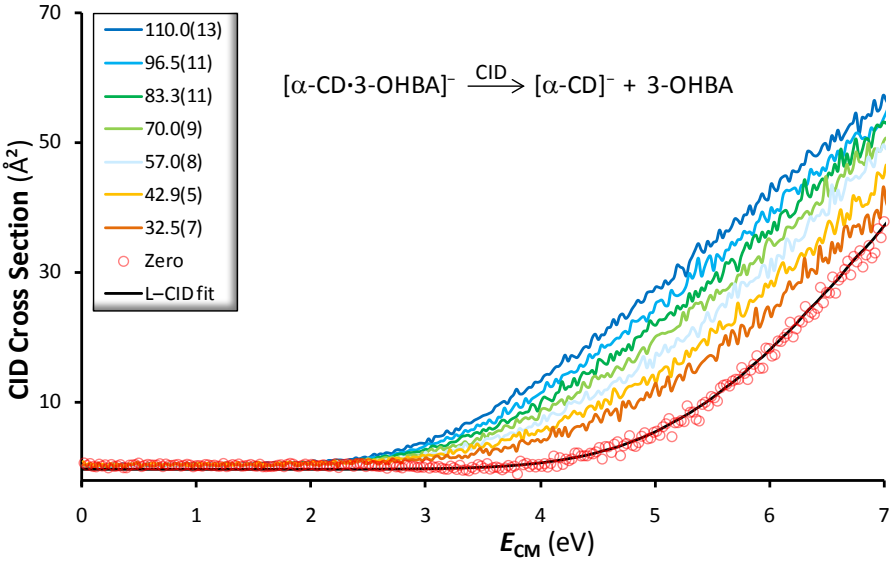


Figure S9. Threshold reactive collision cross-section curves for the dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{3-OHBA}]^-$ at various collision gas pressures, extrapolation to zero pressure, and fitted curve from L-CID assuming no reverse barrier.

Table S1. Fitted parameters and standard deviations (in parentheses) for three independent data sets of the one-channel reactive cross-section curves for dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{3-MeBA}]^-$, assuming either a tight or a loose transition-state model.

			Loose TS			Tight TS		
Data set	V_{cen} (V)	**fwhm** (V)	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})
1	−2.27	1.28	1.715(27)	689(23)	5766(241)	1.144(17)	832(40)	272(120)
2	−2.75	1.20	1.792(17)	878(46)	5661(190)	1.216(18)	946(43)	257(82)
3	−2.58	0.97	1.800(23)	933(35)	5739(241)	1.205(23)	959(39)	258(138)
Average(1—3)			1.77(2)	$8.3(4)\cdot10^2$	$5.7(2)\cdot10^3$	1.19(2)	$9.1(4)\cdot10^2$	$2.6(12)\cdot10^2$

Table S2. Fitted parameters and standard deviations (in parentheses) for three independent data sets of the one-channel reactive cross-section curves for dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{BA}]^-$, assuming either a tight or a loose transition-state model.

			Loose TS			Tight TS		
Data set	V_{cen} (V)	**fwhm** (V)	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})
1	−2.58	1.15	1.725(30)	672(36)	5908(259)	1.121(20)	786(53)	230(110)
2	−2.75	1.63	1.806(14)	791(66)	5918(225)	1.213(19)	903(37)	255(100)
3	−2.69	1.08	1.816(18)	905(34)	5927(166)	1.245(14)	962(30)	288(87)
Average (1–3)			1.78(2)	$7.9(5)\cdot10^2$	$5.9(2)\cdot10^3$	1.193(18)	$8.8(4)\cdot10^2$	$2.6(10)\cdot10^2$

Table S3. Fitted parameters and standard deviations (in parentheses) for three independent data sets of the one-channel reactive cross-section curves for dissociation of $[\alpha\text{-CD}]^-$ from $[\alpha\text{-CD}\cdot\text{3-OHBA}]^-$, assuming either a tight or a loose transition-state model.

			Loose TS			Tight TS		
Data set	V_{cen} (V)	**fwhm** (V)	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})	E_0 (eV)	ν_{eff} (cm^{-1})	α' (cm^{-1})
1	−2.41	1.64	1.768(26)	656(44)	6155(234)	1.159(12)	800(49)	244(103)
2	−2.61	0.93	1.846(15)	909(34)	5570(148)	1.283(21)	968(30)	291(108)
3	−2.57	0.96	1.824(20)	814(40)	5922(170)	1.235(13)	922(37)	284(125)
Average(1–3)			1.81(2)	$7.9(4)\cdot10^2$	$5.88(19)\cdot10^3$	1.226(16)	$9.0(4)\cdot10^2$	$2.7(11)\cdot10^2$

2. DFT Calculations

A detailed investigation of the complexes was performed by means of DFT calculations using the Gaussian 09 program.[8] Basis set superposition errors (BSSEs) were computed with the counterpoise approach.

Table S4. Absolute energies (in Hartree) and basis set superposition errors (BSSEs) for complexes [α-CD·RBA]$^-$.

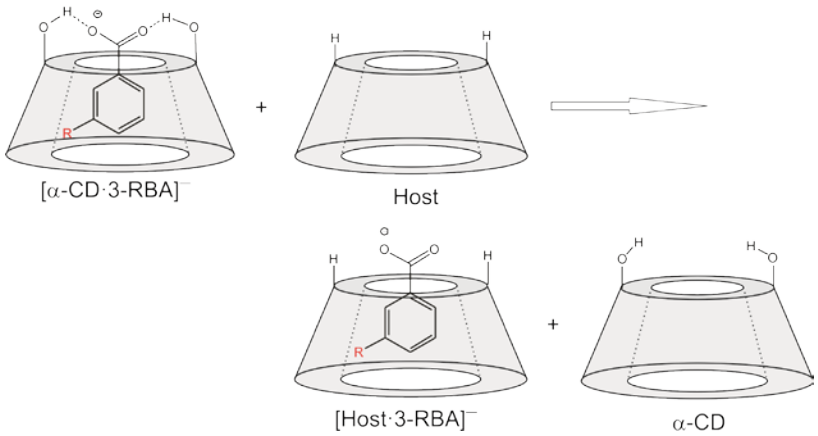
Species[a]	[α-CD·3-MeBA]$^-$	[α-CD·BA]$^-$	[α-CD·3-OHBA]$^-$
BLYP/6-31+G(d,p)			
[α-CD]$^-$	−3663.18531201	−3663.18531201	−3663.18531201
RBA	−460.014613308	−420.720582508	−495.941484822
α-CD	−3663.71994112	−3663.71994112	−3663.71994112
[RBA]$^-$	−459.466215744	−420.173495220	−495.397040720
[α-CD·RBA]$^-$	−4123.22502066	−4083.93146826	−4159.15394097
α-CD$^{\#}$	−3663.66570261	−3663.67042715	−3663.67006507
[RBA]$^{-\#}$	−459.464793865	−420.170230448	−495.393311103
BSSE	0.009318652034	0.008656210341	0.009867986480
M06-L/6-31+G(d,p)			
[α-CD]−	−3663.82007571	−3663.82007571	−3663.82007571
RBA	−460.115526056	−420.800846719	−496.021818825
α-CD	−3664.36214988	−3664.36214988	−3664.36214988
[RBA]−	−459.558313046	−420.244837865	−495.468115442
[α-CD·RBA]−	−4124.01719450	−4084.70035040	−4159.92752294
α-CD#	−3664.31109470	−3664.31669106	−3664.315252
[RBA]−#	−459.556682773	−420.242933666	−495.4652991
BSSE	0.009218065996	0.008224249137	0.009259099
M06-2X//BLYP/6-31+G(d,p)			
[α-CD]−	−3662.85821732	−3662.85821732	−3662.85821732
RBA	−459.969533871	−420.670577221	−495.871660909
α-CD	−3663.39798665	−3663.39798665	−3663.39798665
[RBA]−	−459.416547411	−420.118722143	−495.322762751
[α-CD·RBA]−	−4122.89256455	−4083.59080107	−4158.79774765
α-CD#	−3663.33355452	−3663.33765521	−3663.33760325
[RBA]−#	−459.414967351	−420.113898427	−495.317943114
BSSE	0.009288312026	0.009130876763	0.010140603075
M06-2X//M06-L/6-31+G(d,p)			
[α-CD]−	−3662.90321993	−3662.90321993	−3662.90321993
RBA	−459.9729505	−420.673756421	−495.8754593
α-CD	−3663.44322099	−3663.44322099	−3663.44322099
[RBA]−	−459.4198929	−420.121812816	−495.3265472
[α-CD·RBA]−	−4122.95148442	−4083.65174742	−4158.86003652
α-CD#	−3663.3864701	−3663.39292419	−3663.39082703
[RBA]−#	−459.418099775	−420.119559235	−495.323603519
BSSE	0.010625071694	0.009936538396	0.011312885021

[a] Entries marked with # use the geometries of host or guest in the corresponding host–guest complex.

Table S5. M06-2X//M06-L/6-31+G(d,p) absolute energies (in Hartree) and basis set superposition errors (BSSEs), and hydrogen bond strengths (in kcal mol^{-1}) according to the host-exchange reaction.

Species[a]	Primary	Secondary	Tertiary	All OH groups
[α-CD·3-MeBA]$^-$	–4122.95148443	–4122.95148443	–4122.95148443	–4122.95148443
BSSE	0.01062506952	0.01062506952	0.01062506952	0.01062506952
Host#	–3512.99436525	–3513.01025390	–3512.98914903	–3212.23648113
α-CD#	–3663.38647011	–3663.38647011	–3663.38647011	–3663.38647011
[Host·3-MeBA]$^{-}$#	–3972.52129989	–3972.54706069	–3972.54850882	–3671.72688061
BSSE	0.00913123507	0.00902253961	0.01042333431	0.00731580590
Host–Guest bonding diff.	–23.0	–16.7	–3.4	–44.7
[α-CD·BA]$^-$	–4083.65178621	–4083.65178621	–4083.65178621	–4083.65178621
BSSE	0.00993653840	0.00993653840	0.00993653840	0.00993653840
Host#	–3512.99771321	–3513.00992718	–3512.99141351	–3212.23581125
α-CD#	–3663.39292419	–3663.39292419	–3663.39292419	–3663.39292419
[Host·BA]$^{-}$#	–3933.22205623	–3933.24606177	–3933.24319227	–3632.42859768
BSSE	0.00867568522	0.00850342001	0.00963308652	0.00687985392
Host–Guest bonding diff.	–20.9	–13.4	–4.3	–39.5
[α-CD·3-OHBA]$^-$	–4158.86003652	–4158.86003652	–4158.86003652	–4158.86003652
BSSE	0.01131288502	0.01131288502	0.01131288502	0.01131288502
Host#	–3512.99643706	–3513.00981621	–3512.99047788	–3212.23568863
α-CD#	–3663.39082703	–3663.39082703	–3663.39082703	–3663.39082703
[Host·3-OHBA]$^{-}$#	–4008.43125631	–4008.45473643	–4008.45239195	–3707.63678905
BSSE	0.01002896797	0.00982850079	0.01105692506	0.00811587526
Host–Guest bonding diff.	–20.8	–14.3	–4.4	–40.7

[a] Entries marked with # use geometries derived from the corresponding [α-CD·RBA]$^-$ complex.



Scheme S1. General approach for O–H···O hydrogen bond strength analysis. R = Me, H, OH.

Table S6. M06–2X//M06-L/6-31+G(d,p) absolute energies (in Hartree) and basis set superposition errors (BSSEs), and bond strength (in kcal mol^{-1}) for the *meta*-hydroxyl hydrogen bond in complex **3** as determined from the guest-exchange reaction $[\alpha\text{-CD}\cdot\text{3-OHBA}]^- + BA^- \rightarrow [\alpha\text{-CD}\cdot BA]^- + \text{3-OHBA}^-$.

Species[a]	Energy
$[\alpha\text{-CD}\cdot\text{3-OHBA}]^-$	–4158.86003652
BSSE	0.011312885021
$BA^{-\#}$	–420.11858781
$\text{3-OHBA}^{-\#}$	–495.32360352
$[\alpha\text{-CD}\cdot BA]^{-\#}$	–4083.65033264
BSSE	0.009895552276
Host–Guest bonding diff.	–2.1

[a] Entries marked with # use geometries derived from the corresponding $[\alpha\text{-CD}\cdot RBA]^-$ complex.

Table S7. M06-2X//M06-L distances (Å) and angles (°)[a] and hydrogen bond strengths (kcal mol^{-1}) in complexes **1**–**3**.

	Type	$R_{O\cdots O}$	∠O–H···O	$E_{OH\cdots O}$
1	Primary	2.727	156.94	−23.0
	Secondary	2.898	148.27	−16.7
	Tertiary	4.340	125.85	−3.4
2	Primary	2.827	155.78	−20.9
	Secondary	2.969	139.72	−13.4
	Tertiary	3.386	105.19	−4.3
3	Primary	2.850	155.09	−20.8
	Secondary	2.939	142.85	−14.3
	Tertiary	3.447	106.79	−4.4
	ArOH···OCD	3.359	164.32	−2.1

[a] Values for hydrogen bond pairs are averaged.

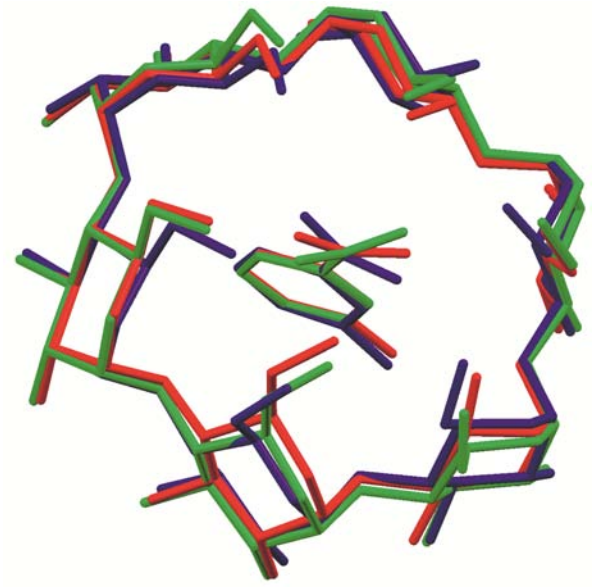


Figure S10. Overlaid structures of complexes **1** (blue), **2** (green), and **3** (red). Hydrogen atoms are omitted for clarity.

Table S8. Bond lengths (Å) for C–H···O ($R_{C\cdots O}$) and C–H···π ($R_{C\cdots\pi}$) hydrogen bonds for calculated geometries and crystal structures of α-CD complexes.

Guest	$R_{C\cdots O}$	$R_{C\cdots\pi}$	Reference
3-MeBA	3.366	4.421	[a]
BA	3.396	4.574	[a]
3-OHBA	3.358	4.583	[a]
4-chlorophenol	3.364	4.319	20d
4-bromophenol	3.356	4.331	20e
4-iodophenol	3.318	4.324	20a
4-hydroxybenzoic acid	3.350	4.281	20a
4-nitrophenol	3.359	4.327	20b
3-nitroaniline	3.422	4.545	20c

[a] This work, M06-L optimizations

3. Additional References

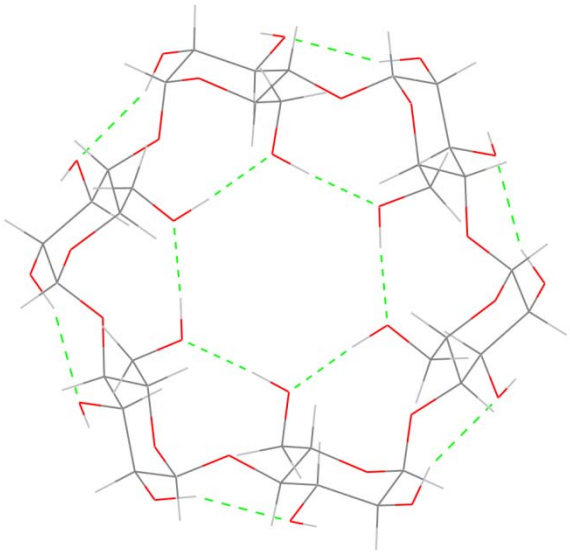
[8] Full reference: Gaussian 09, Revision A.1, M. J Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, 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, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[21] P. B. Armentrout, *J. Am. Soc. Mass Spectrom.*, 2002, **13**, 419–434.

[22] K. M. Ervin and P. B. Armentrout, *J. Chem. Phys.*, 1985, **83**, 166–189.

4. BLYP/6-31+G(d,p) Optimized Geometries

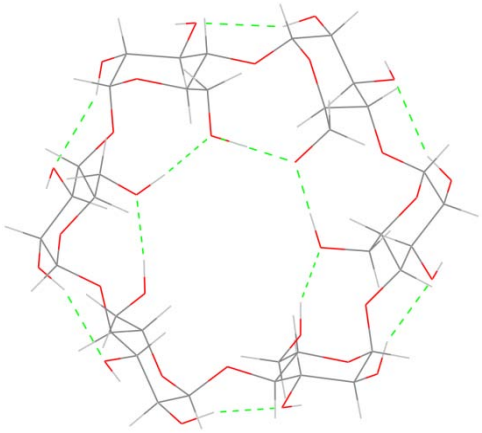
Global minimum conformation for α–CD.



O	0.740962	5.038175	1.191843
C	0.000000	5.414969	0.024212
C	0.967104	5.760700	−1.134089
C	1.939915	4.583010	−1.381596
C	2.643856	4.133641	−0.086291
C	1.584705	3.848519	1.017613
O	−0.848127	4.362844	−0.441872
C	−2.257910	4.356467	−0.086291
C	−2.999045	3.971520	−1.381596
C	−4.505361	3.717886	−1.134089
C	−4.689501	2.707485	0.024212
O	−3.992707	3.160780	1.191843
C	−2.540562	3.296654	1.017613
O	−4.202397	1.446922	−0.441872
C	−4.901766	0.222826	−0.086291
C	−4.938960	−0.611489	−1.381596
C	−5.472464	−2.042814	−1.134089
C	−4.689501	−2.707485	0.024212
O	−4.733669	−1.877396	1.191843
C	−4.125268	−0.551864	1.017613
O	−3.354270	−2.915922	−0.441872
C	−2.643856	−4.133641	−0.086291
C	−1.939915	−4.583010	−1.381596
C	−0.967104	−5.760700	−1.134089
C	0.000000	−5.414969	0.024212
O	−0.740962	−5.038175	1.191843
C	−1.584705	−3.848519	1.017613
O	0.848127	−4.362844	−0.441872
C	2.257910	−4.356467	−0.086291
C	2.999045	−3.971520	−1.381596
C	4.505361	−3.717886	−1.134089
C	4.689501	−2.707485	0.024212
O	3.992707	−3.160780	1.191843
C	2.540562	−3.296654	1.017613
O	4.202397	−1.446922	−0.441872
C	4.901766	−0.222826	−0.086291
C	4.938960	0.611489	−1.381596
C	5.472464	2.042814	−1.134089
C	4.689501	2.707485	0.024212
O	4.733669	1.877396	1.191843
C	4.125268	0.551864	1.017613
O	5.757011	−0.095009	−2.343792
C	4.097558	−0.098217	2.419294
O	2.830444	0.123315	3.090136
O	3.354270	2.915922	−0.441872
O	5.436449	2.821806	−2.343229
O	5.161980	−3.297200	−2.343229
O	2.796225	−5.033222	−2.343792
C	1.963720	−3.597698	2.419294
O	1.522016	−2.389579	3.090136
O	−0.274468	−6.119006	−2.343229
O	−2.960786	−4.938213	−2.343792
C	−2.133838	−3.499481	2.419294
O	−1.308428	−2.512894	3.090136
O	−5.436449	−2.821806	−2.343229
O	−5.757011	0.095009	−2.343792
C	−4.097558	0.098217	2.419294
O	−2.830444	−0.123315	3.090136
O	−5.161980	3.297200	−2.343229
O	−2.796225	5.033222	−2.343792
C	−1.963720	3.597698	2.419294
O	−1.522016	2.389579	3.090136
O	0.274468	6.119006	−2.343229
O	2.960786	4.938213	−2.343792
C	2.133838	3.499481	2.419294
O	1.308428	2.512894	3.090136
H	5.152252	3.661591	0.326129
H	6.534014	1.981552	−0.840878
H	3.902757	0.682460	−1.763348
H	5.930342	−0.459633	0.243478
H	3.084569	0.672675	0.673177
H	4.280965	−1.179138	2.345555
H	4.894173	0.356634	3.031324
H	4.556102	3.262679	−2.404328
H	5.881042	0.513142	−3.102487
H	2.337090	−0.739936	3.111824
H	5.747157	−2.631185	0.326129
H	4.983081	−4.667846	−0.840878
H	2.542406	−3.038656	−1.763348
H	2.567117	−5.365643	0.243478
H	2.124838	−2.334977	0.673177
H	1.119319	−4.296993	2.345555

H	2.755940	−4.060161	3.031324
H	5.103614	−2.314360	−2.404328
H	3.384915	−4.836560	−3.102487
H	0.594905	−6.292777	0.326129
H	−1.550933	−6.649398	−0.840878
H	−1.360350	−3.721116	−1.763348
H	−3.363224	−4.906010	0.243478
H	−0.959730	−3.007652	0.673177
H	−2.138232	−4.416795	3.031324
H	−3.161645	−3.117855	2.345555
H	0.547512	−5.577039	−2.404328
H	−2.496127	−5.349703	−3.102487
H	−1.809349	−1.654011	3.111824
H	−5.152252	−3.661591	0.326129
H	−6.534014	−1.981552	−0.840878
H	−3.902757	−0.682460	−1.763348
H	−5.930342	0.459633	0.243478
H	−3.084569	−0.672675	0.673177
H	−4.556102	−3.262679	−2.404328
H	−5.881042	−0.513142	−3.102487
H	−5.747157	2.631185	0.326129
H	−4.983081	4.667846	−0.840878
H	−2.542406	3.038656	−1.763348
H	−2.567117	5.365643	0.243478
H	−2.124838	2.334977	0.673177
H	−1.119319	4.296993	2.345555
H	−2.755940	4.060161	3.031324
H	−5.103614	2.314360	−2.404328
H	−3.384915	4.836560	−3.102487
H	−0.527742	2.393948	3.111824
H	−0.594905	6.292777	0.326129
H	1.550933	6.649398	−0.840878
H	1.360350	3.721116	−1.763348
H	3.363224	4.906010	0.243478
H	0.959730	3.007652	0.673177
H	3.161645	3.117855	2.345555
H	2.138232	4.416795	3.031324
H	−0.547512	5.577039	−2.404328
H	2.496127	5.349703	−3.102487
H	1.809349	1.654011	3.111824
H	0.527742	−2.393948	3.111824
H	−4.280965	1.179138	2.345555
H	−4.894173	−0.356634	3.031324
H	−2.337090	0.739936	3.111824

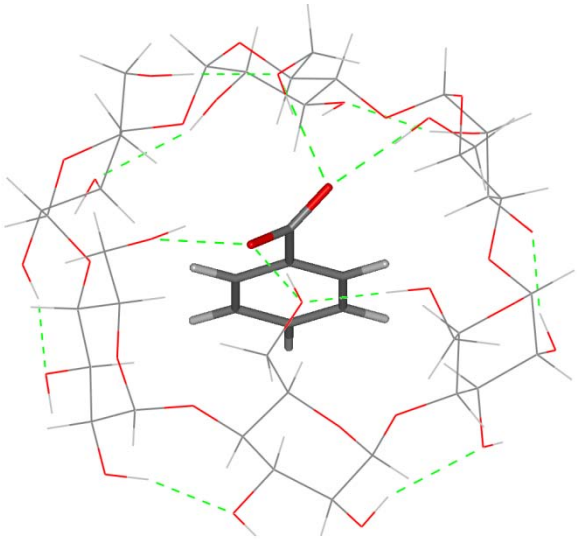
Global minimum conformation for deprotonated α–CD.



C	0.793201	4.649090	1.241971
C	−0.059636	5.194464	0.056540
C	0.850562	5.670656	−1.092182
C	1.898154	4.611298	−1.494651
C	2.662108	4.150668	−0.232202
O	1.738949	3.648705	0.729397
O	−0.828318	6.365017	0.451966
C	−2.254167	6.282361	0.570621
C	−2.873600	7.413609	−0.289407
C	−2.463600	8.781449	0.294991
C	−2.822942	8.895497	1.784383
C	−2.291084	7.669128	2.589710
O	−2.691159	6.422388	1.921829
O	−2.185219	10.133780	2.220222
C	−2.846525	10.991975	3.147382
C	−2.545833	12.444954	2.705858
C	−1.056508	12.787107	2.946823
C	−0.596272	12.441851	4.377844
C	−0.959591	10.959106	4.693027
O	−2.409036	10.796297	4.494225
O	0.841030	12.666872	4.365168
C	1.482982	13.199138	5.528606
C	2.606203	14.140522	5.032171
C	3.763664	13.328523	4.403862
C	4.239978	12.174442	5.312866
C	3.009184	11.301252	5.707177
O	2.033162	12.190286	6.370995
O	5.197490	11.442307	4.500853
C	6.380266	10.902914	5.105969
C	7.483606	10.950527	4.020985
C	7.188135	9.918752	2.908143
C	6.887020	8.513318	3.471690
C	5.748980	8.623075	4.527412
O	6.215617	9.567487	5.567838
O	6.469679	7.732899	2.315144
C	6.987765	6.416663	2.116889

O	6.182212	5.397167	2.708108
C	4.772415	5.442894	2.280095
C	4.734877	5.126536	0.759656
C	5.615405	6.145307	0.006871
C	7.048721	6.210470	0.582712
O	7.828132	7.228242	−0.083694
O	5.637884	5.787055	−1.402657
O	3.395877	5.292553	0.224923
C	3.973395	4.502245	3.227476
O	2.897175	5.179549	3.879235
O	8.306234	9.825618	1.984711
O	7.656592	12.273664	3.465403
C	5.252724	7.333719	5.266774
O	3.852081	7.197266	5.210511
O	4.892781	14.193450	4.117260
O	2.119005	15.139572	4.110543
C	3.222822	10.100285	6.672002
O	2.424901	8.971201	6.312164
O	−0.813919	14.198498	2.713158
O	−2.912816	12.690486	1.332375
C	−0.667445	10.439364	6.122377
O	−0.327957	9.041105	6.129846
O	−3.114500	9.866792	−0.417984
O	−2.537199	7.333459	−1.687201
C	−2.842204	7.570246	4.036109
O	−1.950622	6.910600	4.939974
O	0.009662	6.007502	−2.233767
O	2.766297	5.116164	−2.532308
C	−0.036410	3.959233	2.345078
O	0.753747	3.444120	3.418346
H	3.345179	3.312737	−0.453734
H	1.379790	3.737571	−1.924167
H	1.376231	6.580381	−0.751718
H	−0.743652	4.406314	−0.311898
H	1.365796	5.479430	1.686822
H	−0.791010	4.682918	2.707097
H	−0.567982	3.092807	1.910255
H	3.560382	5.515419	−2.101768
H	0.623731	6.204476	−2.971703
H	−2.614344	5.291954	0.245448
H	−3.971643	7.315685	−0.238924
H	−1.367372	8.891166	0.201494
H	−3.920124	8.989948	1.896342
H	−1.190301	7.721431	2.622796
H	−3.089498	8.578449	4.404481
H	−3.771254	6.974513	3.994503
H	−1.600953	7.023096	−1.784009
H	−3.017359	9.648072	−1.369058
H	−3.931958	10.793451	3.157906
H	−3.166492	13.124946	3.313416
H	−0.439574	12.191083	2.248114
H	−1.072016	13.125249	5.106772
H	−0.422943	10.312730	3.979565
H	−1.582371	10.574916	6.725600
H	0.145546	11.020835	6.579052
H	−2.728140	11.866670	0.821546
H	−1.224286	14.399100	1.846153
H	0.674744	8.960095	6.184375
H	0.753609	13.743716	6.153271
H	2.997543	14.693921	5.902352
H	3.404581	12.875471	3.460135
H	4.743106	12.574882	6.213580
H	2.560572	10.904876	4.782011
H	1.418539	14.715250	3.561350
H	4.522571	14.965828	3.641125
H	6.660899	11.496925	5.993566
H	8.444108	10.692925	4.497939
H	6.289677	10.247475	2.352399
H	7.797253	8.067200	3.914118
H	4.866560	9.054532	4.029622
H	5.756150	6.453081	4.822319
H	5.630673	7.415796	6.312706
H	6.765907	12.694779	3.440267
H	8.535066	10.748951	1.749266
H	3.270177	5.969715	4.456866
H	7.983810	6.314418	2.581246
H	7.558320	5.253014	0.382109
H	5.143549	7.139126	0.116771
H	5.089197	4.096037	0.569239
H	4.389978	6.464047	2.431238
H	3.531912	3.661261	2.669365
H	4.694720	4.085670	3.958461
H	7.724074	8.061866	0.432432
H	6.295325	6.381558	−1.820483
H	1.373346	4.151997	3.742137
H	−1.357461	7.592940	5.344464
H	4.287026	9.820768	6.687794
H	2.946976	10.443745	7.687964
H	3.045607	8.207168	5.847283

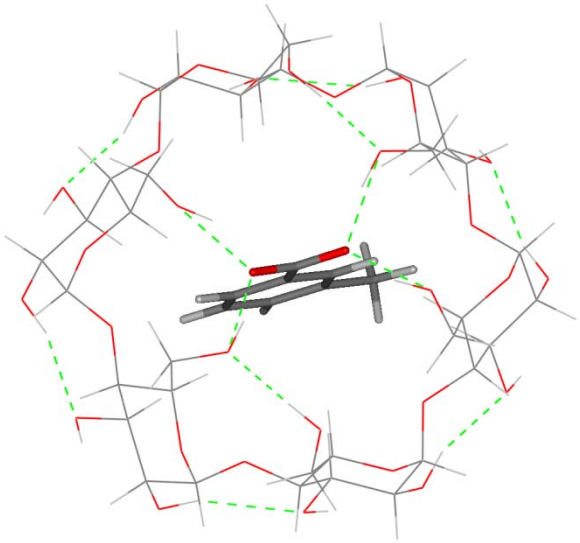
Global minimum conformation for the head orientation of [α–CD·BA]$^-$.



O	0.943668	5.346175	1.327255
C	0.049938	5.563227	0.236932
C	0.869200	5.835564	−1.048892
C	1.805577	4.639205	−1.328988
C	2.698512	4.303665	−0.122958
C	1.872993	4.211626	1.200114
O	−0.801702	4.436309	−0.020398
C	−2.228706	4.476994	0.287393
C	−2.944519	4.057420	−1.010286
C	−4.447699	3.771633	−0.800239
C	−4.620906	2.751642	0.353811
O	−4.005732	3.267079	1.532092
C	−2.550477	3.464249	1.425304
O	−4.040978	1.514722	−0.089176
C	−4.738137	0.256429	0.105260
C	−4.706258	−0.458702	−1.262265
C	−5.284312	−1.892932	−1.193339
C	−4.633259	−2.703277	−0.041776
O	−4.698400	−1.952889	1.172171
C	−4.006970	−0.653389	1.135624
O	−3.297432	−3.009976	−0.448219
C	−2.698661	−4.302576	−0.115867
C	−1.808097	−4.638679	−1.323488
C	−0.871153	−5.834890	−1.044710
C	−0.049378	−5.561978	0.239393
O	−0.940953	−5.344424	1.331374
C	−1.870542	−4.209948	1.205541
O	0.801788	−4.435202	−0.020124
C	2.229360	−4.475736	0.285072
C	2.942841	−4.056633	−1.014063
C	4.446381	−3.770750	−0.806788
C	4.621614	−2.750303	0.346556
O	4.008546	−3.265284	1.526139
C	2.553125	−3.462588	1.422037
O	4.040873	−1.513551	−0.095871
C	4.738372	−0.255173	0.096702
C	4.704185	0.459263	−1.271121
C	5.282338	1.893549	−1.203900
C	4.633257	2.704461	−0.051601
O	4.700477	1.954656	1.162603
C	4.008921	0.655171	1.127811
O	5.452554	−0.339694	−2.228247
C	3.951028	0.156350	2.583064
O	2.863371	0.771509	3.309282
O	3.296734	3.010956	−0.455882
O	5.158409	2.556384	−2.479597
O	5.058404	−3.349116	−2.042775
O	2.748417	−5.107693	−2.002965
C	2.058224	−3.898438	2.812602
O	2.089808	−2.827730	3.768253
O	−0.057902	−6.123501	−2.199556
O	−2.669154	−4.911411	−2.460339
C	−2.745749	−4.247968	2.485894
O	−2.158827	−3.574872	3.602398
O	−5.162542	−2.556411	−2.468913
O	−5.456261	0.339795	−2.218499
C	−3.946713	−0.153972	2.590589
O	−2.857755	−0.768703	3.315255
O	−5.061879	3.349498	−2.034994
O	−2.751838	5.108082	−1.999946
C	−2.052990	3.900531	2.814799
O	−2.082989	2.830228	3.770914
O	0.053714	6.123760	−2.202261
O	2.664377	4.911430	−2.467664
C	2.750707	4.250181	2.478733
O	2.165719	3.577973	3.596787
H	5.198177	3.631898	0.145378
H	6.364358	1.823154	−1.001177
H	3.647657	0.511559	−1.592041
H	5.782655	−0.445294	0.409248
H	2.976952	0.805949	0.774624
H	3.845174	−0.939040	2.609158
H	4.882873	0.436677	3.101310
H	4.281743	3.007522	−2.490406
H	5.483824	0.185685	−3.054844
H	2.039143	0.280744	3.042950
H	5.686063	−2.609244	0.600548
H	4.957238	−4.704696	−0.517310
H	2.463076	−3.130947	−1.375794
H	2.522400	−5.504840	0.567147
H	2.085814	−2.497702	1.174238
H	1.038869	−4.313216	2.715885
H	2.722773	−4.685602	3.208329
H	4.980950	−2.365718	−2.115976
H	3.314125	−4.864187	−2.765973
H	0.553940	−6.440320	0.524910
H	−1.481030	−6.738169	−0.871354

H	−1.190310	−3.750924	−1.542758
H	−3.498454	−5.062673	−0.024373
H	−1.290923	−3.273258	1.185472
H	−2.870474	−5.307922	2.768396
H	−3.738398	−3.825511	2.261672
H	0.789132	−5.614899	−2.140872
H	−2.077672	−5.267738	−3.156355
H	−2.408743	−2.617540	3.544443
H	−5.197821	−3.630630	0.156622
H	−6.365979	−1.822428	−0.988785
H	−3.650279	−0.511158	−1.584968
H	−5.781907	0.446733	0.419404
H	−2.975554	−0.804233	0.780840
H	−4.285893	−3.007558	−2.480982
H	−5.488947	−0.185994	−3.044779
H	−5.684903	2.610698	0.609764
H	−4.958045	4.705701	−0.510254
H	−2.465407	3.131575	−1.372491
H	−2.521219	5.506198	0.569646
H	−2.083699	2.499233	1.177012
H	−1.033747	4.315119	2.716024
H	−2.716655	4.687978	3.211456
H	−4.984497	2.366080	−2.107937
H	−3.318916	4.864293	−2.761847
H	−1.446487	2.144815	3.462936
H	−0.552831	6.441689	0.523234
H	1.479455	6.738885	−0.877096
H	1.187370	3.751342	−1.546643
H	3.498450	5.063833	−0.033369
H	1.293316	3.274933	1.181616
H	3.742815	3.827305	2.252856
H	2.876284	5.310268	2.760347
H	−0.793337	5.615418	−2.141599
H	2.071505	5.267473	−3.162643
H	2.414897	2.620461	3.538778
H	1.452271	−2.142790	3.461393
H	−3.841021	0.941449	2.616110
H	−4.877633	−0.434289	3.110492
H	−2.033979	−0.278075	3.047235
C	0.222355	−1.193501	−2.222298
C	0.237649	−1.188658	−0.815168
C	−0.000079	0.000483	−0.091985
C	−0.239040	1.189170	−0.815501
C	−0.226167	1.193115	−2.222657
C	−0.002534	−0.000420	−2.935118
H	0.391267	−2.128935	−2.764113
H	0.418106	−2.115134	−0.272688
H	−0.418563	2.116004	−0.273325
H	−0.396004	2.128212	−2.764767
H	−0.003497	−0.000758	−4.029136
C	0.001118	0.000861	1.442971
O	0.877009	−0.729877	2.025289
O	−0.873894	0.731956	2.026256

Global minimum conformation for the head orientation of [α–CD·3–MeBA]$^-$.

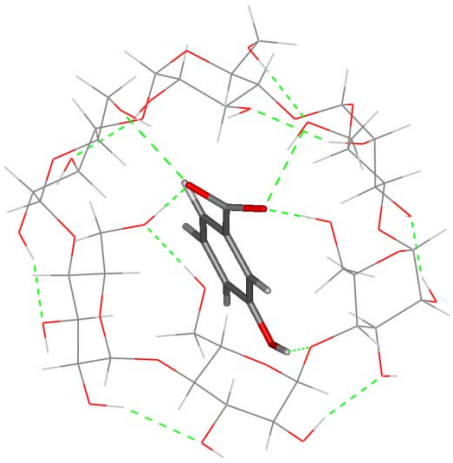


O	0.792279	4.981359	1.592508
C	0.036338	5.398756	0.461705
C	0.999176	5.773993	−0.694918
C	1.920579	4.573875	−1.012536
C	2.651178	4.039210	0.233977
C	1.626379	3.784169	1.376733
O	−0.833383	4.373160	−0.046483
C	−2.269994	4.391055	0.188364
C	−2.898925	4.109354	−1.194392
C	−4.421683	3.840590	−1.142359
C	−4.755391	2.784549	−0.056886
O	−4.166118	3.185900	1.183306
C	−2.696939	3.248487	1.157278
O	−4.270950	1.526430	−0.530837
C	−5.023655	0.296039	−0.291099
C	−4.703119	−0.597010	−1.502070
C	−5.260861	−2.026534	−1.314976
C	−4.731622	−2.633219	0.008249
O	−5.090618	−1.779265	1.094792
C	−4.591612	−0.395556	1.041315
O	−3.315687	−2.814543	−0.123697
C	−2.695073	−4.066914	0.297580
C	−1.979926	−4.632574	−0.943330
C	−1.051550	−5.822880	−0.609544
C	−0.075460	−5.419758	0.525640
O	−0.820547	−4.975895	1.653219
C	−1.652328	−3.781176	1.415516
O	0.791531	−4.409596	−0.017015
C	2.229145	−4.427836	0.216963
C	2.853957	−4.156737	−1.169231
C	4.376812	−3.889169	−1.128219
C	4.714109	−2.823311	−0.054140
O	4.132910	−3.215932	1.191327

C	2.662680	−3.281482	1.177116
O	4.223765	−1.570320	−0.537019
C	4.974277	−0.335887	−0.311602
C	4.645124	0.546210	−1.527848
C	5.206381	1.976299	−1.356685
C	4.683460	2.595597	−0.036446
O	5.046907	1.751322	1.056292
C	4.549522	0.366074	1.017942
O	5.205604	−0.082162	−2.710747
C	5.121804	−0.305322	2.294103
O	4.311645	−0.107678	3.456021
O	3.266821	2.776642	−0.161806
O	4.925555	2.775019	−2.523132
O	4.859193	−3.521753	−2.438819
O	2.552169	−5.284694	−2.035994
C	2.216947	−3.380701	2.646375
O	2.221433	−2.080824	3.279176
O	−0.377425	−6.293666	−1.796149
O	−2.987221	−5.019289	−1.919635
C	−2.262807	−3.390455	2.771400
O	−1.281345	−2.865696	3.679369
O	−4.981835	−2.835818	−2.475147
O	−5.273218	0.020838	−2.685588
C	−5.152826	0.286922	2.316179
O	−4.337004	0.090966	3.474616
O	−4.912155	3.462431	−2.446448
O	−2.605372	5.234327	−2.069089
C	−2.233830	3.352043	2.621262
O	−2.236126	2.056279	3.261926
O	0.312123	6.218787	−1.883645
O	2.918699	4.938871	−2.007339
C	2.257844	3.432969	2.734788
O	1.294888	2.906080	3.661268
H	5.175257	3.560788	0.172562
H	6.306542	1.916438	−1.284292
H	3.545926	0.600874	−1.627233
H	6.057391	−0.565598	−0.302625
H	3.448148	0.378435	1.067165
H	5.269302	−1.381282	2.111015
H	6.104381	0.155510	2.495831
H	4.119827	3.323816	−2.357978
H	5.113628	0.582566	−3.425487
H	3.613767	−0.812500	3.456023
H	5.801423	−2.771861	0.127336
H	4.899678	−4.822448	−0.860863
H	2.363717	−3.252685	−1.571378
H	2.537936	−5.418117	0.601478
H	2.263258	−2.340540	0.770921
H	1.210878	−3.825271	2.712652
H	2.925586	−4.011307	3.207521
H	4.731589	−2.548147	−2.531513
H	3.026808	−5.115147	−2.876495
H	0.514092	−6.284049	0.876392
H	−1.662422	−6.668670	−0.251036
H	−1.369514	−3.818751	−1.369420
H	−3.472766	−4.772390	0.646658
H	−0.998457	−2.961777	1.079291
H	−2.684898	−4.285842	3.259037
H	−3.080344	−2.667122	2.604348
H	0.471074	−5.796162	−1.891552
H	−2.503766	−5.485784	−2.633692
H	−0.889223	−2.067201	3.256515
H	−5.221745	−3.596698	0.228548
H	−6.360821	−1.968101	−1.238793
H	−3.604523	−0.650669	−1.608885
H	−6.106033	0.528626	−0.277617
H	−3.489941	−0.409293	1.082033
H	−4.182169	−3.390224	−2.301454
H	−5.179750	−0.646074	−3.397914
H	−5.841728	2.737739	0.131297
H	−4.942596	4.776479	−0.879997
H	−2.407050	3.205376	−1.595581
H	−2.580374	5.382303	0.568749
H	−2.306827	2.304026	0.750309
H	−1.225945	3.794035	2.673770
H	−2.933749	3.988604	3.186740
H	−4.778964	2.489191	−2.534699
H	−3.085945	5.059607	−2.905201
H	−1.462598	1.557409	2.880864
H	−0.551621	6.269946	0.797606
H	1.616397	6.626221	−0.363269
H	1.304914	3.751906	−1.415660
H	3.433155	4.754469	0.552678
H	0.974151	2.949900	1.078119
H	3.087799	2.722443	2.573902
H	2.665857	4.346530	3.200226
H	−0.537410	5.719307	−1.960984
H	2.427070	5.383365	−2.729787
H	0.933946	2.077545	3.269119
H	1.458041	−1.582334	2.876086
H	−5.295166	1.362533	2.127378
H	−6.136733	−0.167039	2.526488
H	−3.632951	0.789197	3.464181
C	0.098138	−1.075104	−2.646904
C	0.123014	−1.129605	−1.234933
C	−0.019298	0.035100	−0.443533
C	−0.190260	1.272810	−1.096351
C	−0.217598	1.345274	−2.500408
C	−0.074990	0.180705	−3.271952
H	0.254804	−2.086784	−0.729735
H	−0.301901	2.172796	−0.497237
H	−0.349403	2.312328	−2.995639
H	−0.097293	0.243183	−4.365468
C	0.263415	−2.325434	−3.502373
H	1.184818	−2.274472	−4.109753
H	0.320143	−3.235488	−2.889258
H	−0.579303	−2.444235	−4.205769
C	0.012548	−0.024685	1.094988

O	0.191725	−1.171177	1.639218
O	−0.139312	1.079624	1.728459

Global minimum conformation for the head orientation of [α–CD·3–OHBA]⁻.



O	0.659297	5.025708	1.226647
C	−0.025630	5.365510	0.019498
C	1.000166	5.563225	−1.127600
C	1.967799	4.358606	−1.223920
C	2.603070	4.000828	0.136444
C	1.451941	3.786751	1.161090
O	−0.950043	4.362917	−0.408724
C	−2.371044	4.477141	−0.080196
C	−3.100434	3.889677	−1.300369
C	−4.606566	3.672336	−1.031334
C	−4.789874	2.814033	0.244530
O	−4.156940	3.461322	1.346746
C	−2.707415	3.691922	1.227610
O	−4.246202	1.515082	−0.030445
C	−4.990859	0.297935	0.280623
C	−4.972250	−0.538754	−1.012706
C	−5.484338	−1.980274	−0.796817
C	−4.700809	−2.636251	0.368252
O	−4.843421	−1.836944	1.540320
C	−4.281009	−0.480521	1.426955
O	−3.337571	−2.764630	−0.065442
C	−2.598007	−3.991872	0.163833
C	−1.972469	−4.367595	−1.196645
C	−1.017896	−5.581924	−1.091579
C	0.020361	−5.378339	0.042741
O	−0.647550	−5.015936	1.251207
C	−1.439755	−3.775680	1.180446
O	0.950618	−4.390215	−0.411978
C	2.369918	−4.498586	−0.078035
C	3.101365	−3.952916	−1.317500
C	4.602538	−3.694279	−1.052236
C	4.773954	−2.797114	0.196575
O	4.143679	−3.407444	1.315856
C	2.698789	−3.670568	1.204741
O	4.238089	−1.498884	−0.129532
C	4.978914	−0.281047	0.216029
C	4.962068	0.578049	−1.060930
C	5.497121	2.008896	−0.828261
C	4.711283	2.649500	0.344729
O	4.854321	1.831778	1.504973
C	4.278172	0.482414	1.378467
O	5.724785	−0.114621	−2.087441
C	4.416634	−0.189237	2.756770
O	3.527537	0.376223	3.731754
O	3.349305	2.775795	−0.088959
O	5.437837	2.776661	−2.045810
O	5.247159	−3.160801	−2.227921
O	2.922338	−4.900667	−2.399702
C	2.309588	−4.396355	2.520056
O	2.021311	−3.508190	3.601569
O	−0.395647	−5.858965	−2.363435
O	−3.046368	−4.648946	−2.135216
C	−1.837597	−3.436758	2.628714
O	−0.762223	−2.773879	3.330817
O	−5.418883	−2.733160	−2.025318
O	−5.772319	0.149752	−2.015624
C	−4.416391	0.176948	2.811900
O	−3.510906	−0.382233	3.776410
O	−5.257845	3.117934	−2.191949
O	−2.901079	4.789307	−2.422797
C	−2.299967	4.443786	2.522861
O	−1.993786	3.577113	3.618207
O	0.362918	5.812415	−2.397483
O	3.035922	4.641598	−2.169542
C	1.858653	3.456389	2.608692
O	0.786783	2.798886	3.320779
H	5.125995	3.634211	0.619748
H	6.562544	1.962293	−0.546431
H	3.913703	0.674169	−1.392470
H	6.019144	−0.548485	0.481363
H	3.206911	0.578729	1.144656
H	4.246106	−1.274638	2.649102
H	5.439121	−0.029120	3.140188
H	4.550748	3.210938	−2.105526
H	5.791394	0.510671	−2.840106
H	2.610753	0.154009	3.451371
H	5.836633	−2.703132	0.476971
H	5.097297	−4.658455	−0.844808
H	2.613886	−3.002051	−1.591899
H	2.633459	−5.564149	0.066042
H	2.165224	−2.708349	1.143839
H	1.450604	−5.058984	2.328803
H	3.172451	−5.016269	2.820843
H	5.257748	−2.174402	−2.176288
H	3.457884	−4.558651	−3.145767
H	0.545475	−6.322015	0.270216
H	−1.616663	−6.475054	−0.845135

H	−1.402060	−3.489809	−1.552481
H	−3.283022	−4.789136	0.509536
H	−0.804562	−2.961022	0.798355
H	−2.052119	−4.370204	3.174755
H	−2.737854	−2.803609	2.642146
H	0.433487	−5.327585	−2.404877
H	−2.614110	−4.966851	−2.955203
H	−0.784078	−1.821695	3.038192
H	−5.118571	−3.623865	0.628495
H	−6.550557	−1.947707	−0.515224
H	−3.927017	−0.592276	−1.362517
H	−6.031468	0.556632	0.554400
H	−3.210761	−0.564224	1.184371
H	−4.535624	−3.174633	−2.079107
H	−5.834692	−0.466468	−2.775660
H	−5.853930	2.733317	0.524898
H	−5.084948	4.650997	−0.854882
H	−2.637050	2.915108	−1.531439
H	−2.635957	5.546720	0.027726
H	−2.192326	2.718572	1.190908
H	−1.445705	5.105720	2.308674
H	−3.159667	5.066525	2.825895
H	−5.231246	2.130321	−2.139549
H	−3.495118	4.461710	−3.130446
H	−1.037642	3.325104	3.547687
H	−0.555568	6.308328	0.239235
H	1.591068	6.466794	−0.900793
H	1.404813	3.471926	−1.569124
H	3.286026	4.804425	0.470983
H	0.815957	2.968626	0.787906
H	2.758600	2.822504	2.620408
H	2.076825	4.392734	3.148261
H	−0.460546	5.270632	−2.423521
H	2.597587	4.938947	−2.993966
H	0.800862	1.847236	3.028055
H	1.060600	−3.268015	3.546634
H	−4.261455	1.265568	2.709978
H	−5.432923	0.000206	3.203508
H	−2.599715	−0.148962	3.487928
C	−0.036913	0.003629	−2.981535
C	1.113484	−0.389308	−2.271079
C	1.128206	−0.376784	−0.862757
C	−0.020008	0.008071	−0.138840
C	−1.177239	0.391637	−0.849524
C	−1.174472	0.399471	−2.257071
H	−0.024043	−0.003539	−4.074053
H	2.026733	−0.677133	−0.324540
H	−2.065927	0.698576	−0.302904
H	−2.069907	0.715543	−2.800511
O	2.219642	−0.780416	−3.022492
H	2.955173	−0.997328	−2.414211
C	−0.000620	0.008841	1.397375
O	1.091313	0.359004	1.969176
O	−1.077658	−0.341059	1.995274