Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Identification and Interconversion of Diastereomeric Oligo-Tröger Bases Probed by Ion Mobility Mass Spectrometry

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Supplementary material

The influence of several parameters on the separation in IM-MS

The effect of the following parameters was investigated: BIAS, IMS gas flow, He gas flow and Trap gas flow. A roughly 1:1 mixture of *syn*-**2** and *anti*-**2** was used with added Na_2SO_4 in MeOH:H_2O (1:1). The sodiated species (*m/z* = 489) was mass selected and the mobility traces were recorded at several parameter sets. Only one parameter was varied at a time.

Figure S1 depicts the IM-MS traces obtained at different value of BIAS parameter, while Figure S2 shows the intensity as function of BIAS. It can be deduced that BIAS has no effect on the separation but strongly influences the intensity.

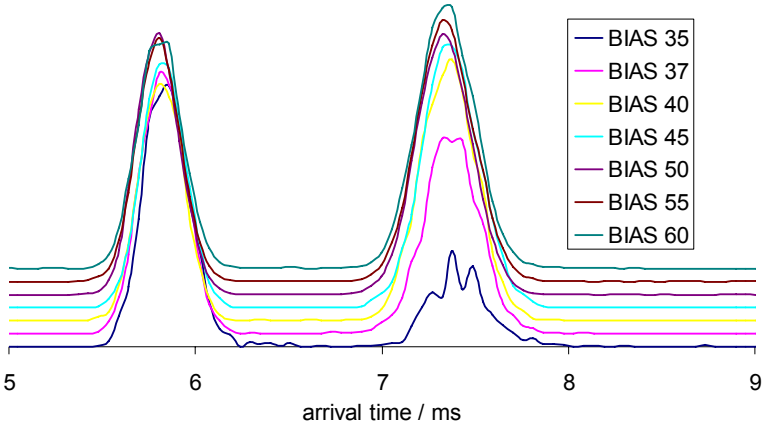


Figure S1. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different BIAS parameters.

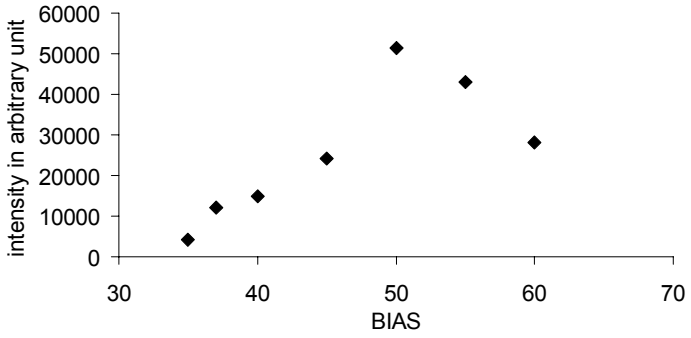


Figure S2. The intensity as a function of BIAS parameter (other parameters were kept constant).

The effect of IMS gas flow was investigated in two different ways: first, only the IMS gas flow was varied (which resulted in the change of the arrival times). Secondly, the IMS gas flow was varied and at any value of IMS gas flow the wave velocity parameter was adjusted in order to have approximately the same arrival times. The IM-MS traces and separation obtained at different value of IMS gas flow without adjusting the wave velocity are shown in Figure S3 and Figure S4. Figure S5 and Figure S6 depict the results for the wave velocity adjusted measurements. As it is expected, the IMS gas flow strongly influences the arrival times (provided the wave velocity is not changed)

as well as the separation between the two forms (both with and without wave velocity adjustment). A closer look reveals that the separation is more or less constant above 60 mL/min, but below that value the separation decreases significantly.

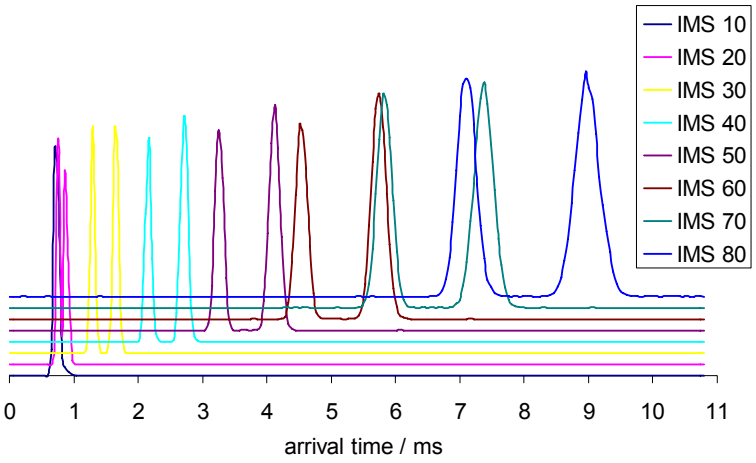


Figure S3. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different values of IMS gas flow (wave velocity was constant).

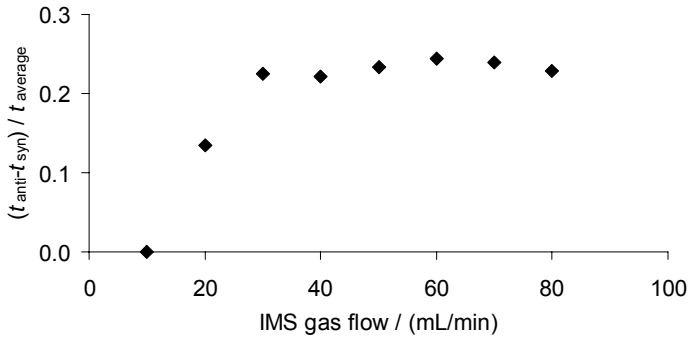


Figure S4. The separation between the two forms as a function of IMS gas flow (wave velocity was constant). The separation is expressed as the arrival time difference of *syn* and *anti* forms divided by their average arrival time ($t_{average}$ = (t_{syn} + t_{anti}) / 2).

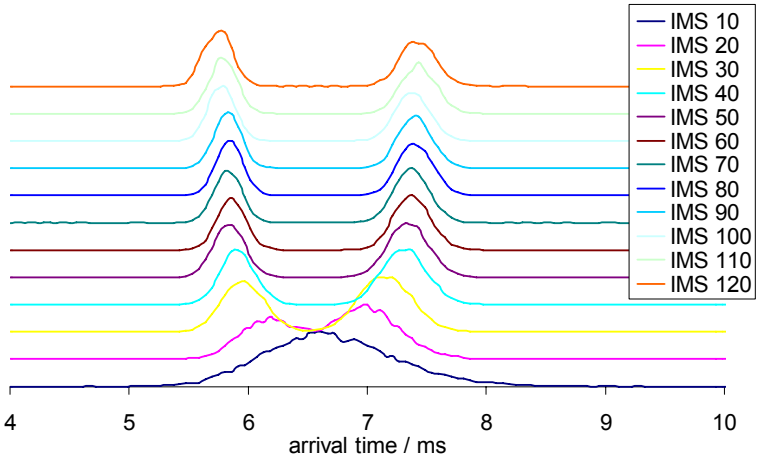


Figure S5. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different values of IMS gas flow (wave velocity was adjusted).

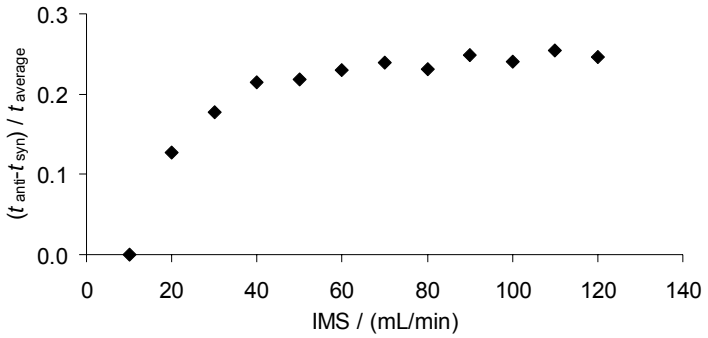


Figure S6. The separation between the two forms as a function of IMS gas flow (wave velocity was adjusted). The separation is expressed as the arrival time difference of *syn* and *anti* forms divided by their average arrival time ($t_{average}$ = (t_{syn} + t_{anti}) / 2).

The effect of He gas flow was investigated analogously to the influence of IMS gas flow. Again, two different methods were used: one is with constant wave velocity and another one with the adjustment of that parameter to get the same arrival times for all the values of He gas flow. The results can be seen in Figure S7, Figure S8 and Figure S9. We can conclude that He gas flow has no effect on the separation, although it influences the arrival time when constant wave velocity is used.

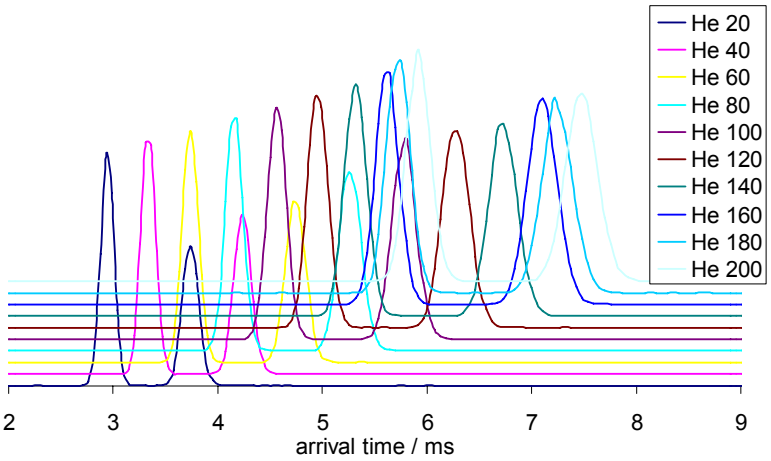


Figure S7. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different values of He gas flow (wave velocity was constant).

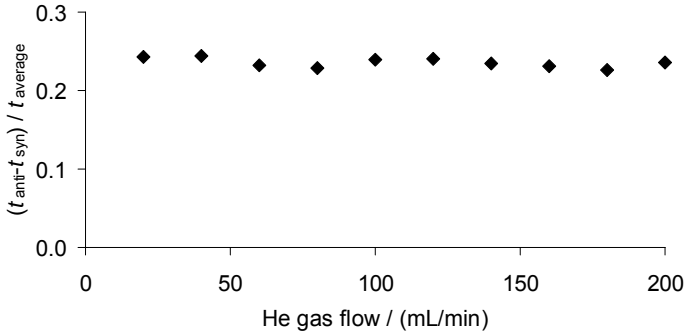


Figure S8. The separation between the two forms as a function of He gas flow (wave velocity was constant).

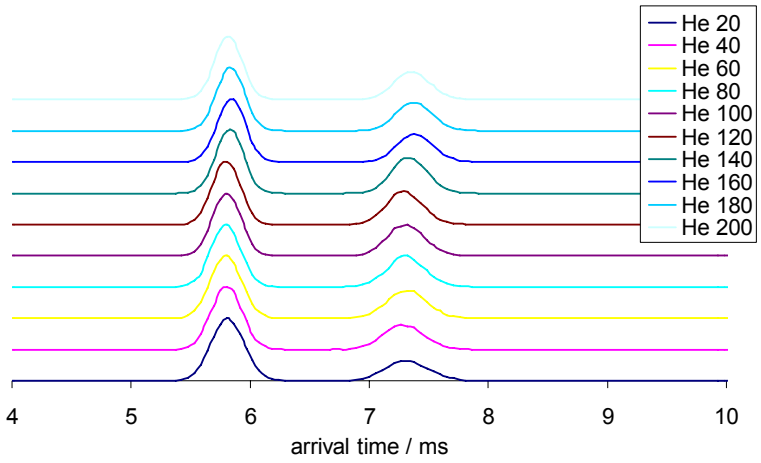


Figure S9. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different values of He gas flow (wave velocity was adjusted).

Finally, the effect of Trap gas flow was studied (see Figure S10 and S11). The investigations revealed that this parameter has influence neither on the arrival times and therefore nor on the separation but slightly influences the intensity.

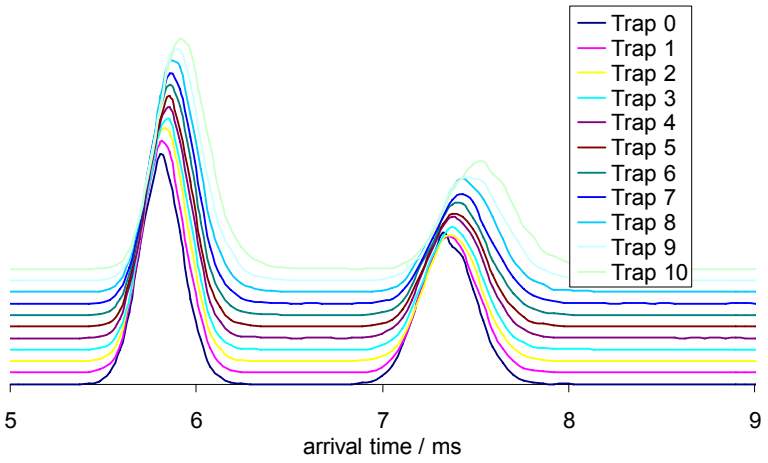


Figure S10. The ion-mobility traces of the mass-selected sodiated ions (**2**Na^+, *m/z* 489) obtained at different values of Trap gas flow.

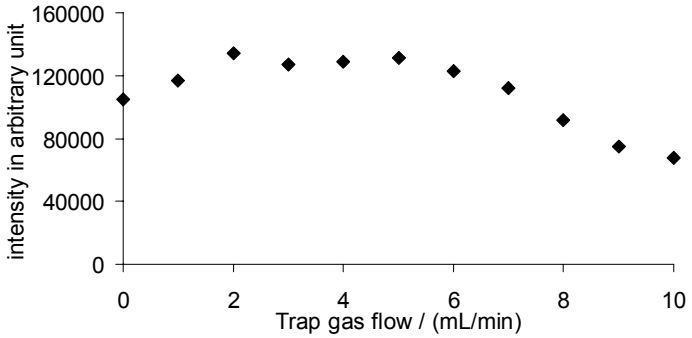


Figure S11. The intensity as a function of Trap gas flow (other parameters were kept constant).

Collisional activation of $1Ag^+$ species

Figure S12 and Figure S13 show the ion-mobility traces for mass-selected *syn*-**1**Ag^+ as well as for *anti*-**1**Ag^+ at different voltages applied to the ion trap in front of the ion-mobility device. Similarly to the sodiated species, the argentated ions have only one peak (at 6.1 ms for *syn*-**1**Ag^+ and at 7.1 ms for *anti*-**1**Ag^+) even at elevated voltages, indicating that **1**Ag^+ does not undergo epimerization. The fast component at 4.6 ms in the IM-MS trace of *anti*-**1**Ag^+ at low voltage comes from the dimer (see main text), while the peak at 7.3 ms appearing at large voltage is due to AgH loss.

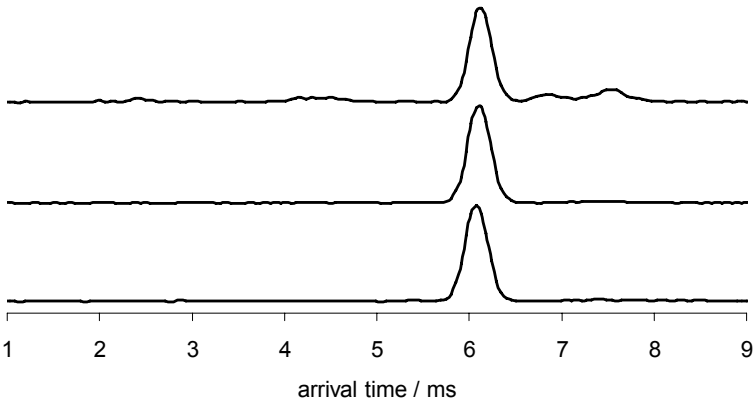


Figure S12. Ion-mobility traces of the mass-selected argentated ion *syn*-**1**Ag^+ (*m/z* 573) at different voltages (U_{tr}) applied to the ion trap in front of the ion-mobility device. The larger U_{tr}, the more the ions are heated in multiple collisions. U_{tr} from bottom to top: 10 V, 20 V, and 40 V.

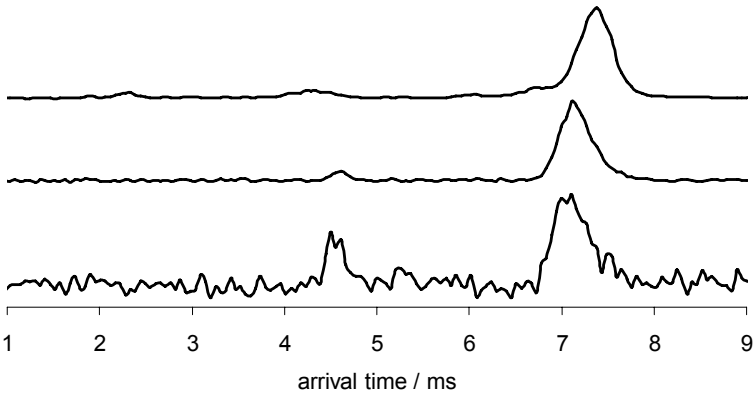


Figure S13. Ion-mobility traces of the mass-selected argentated ion *anti*-**1**Ag^+ (*m/z* 573) at different voltages (U_{tr}) applied to the ion trap in front of the ion-mobility device. The larger U_{tr}, the more the ions are heated in multiple collisions. U_{tr} from bottom to top: 4 V, 20 V, and 40 V.

Collision-induced isomerization of $2H^+$ in the trap prior to the IM unit

The investigation of the effect of the voltage applied to the ion trap was performed with mass-selected *syn*-**2**H^+ and *anti*-**2**H^+. The findings are in agreement with those for activation by cone voltage in the ESI source (see Figure 2 in the full text): isomerization and fragmentation take place at elevated voltages. The exact ratio of the areas of the two peaks was derived from fitting with Gaussian functions.

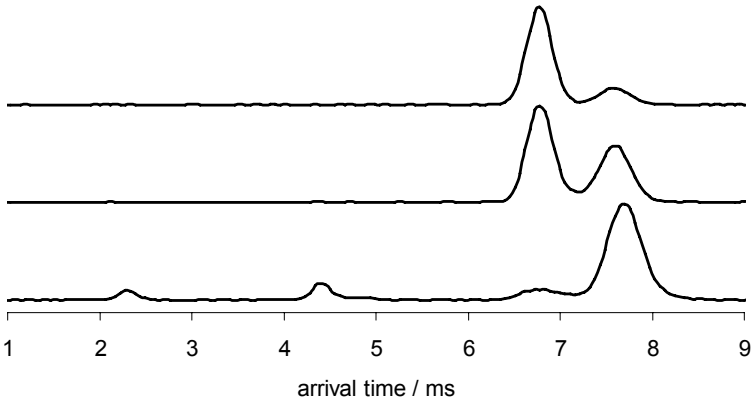


Figure S14. Ion-mobility traces of the mass-selected protonated ion *syn*-**2**H^+ (*m/z* 467) at different voltages (U_{tr}) applied to the ion trap in front of the ion-mobility device. The larger U_{tr}, the more the ions are heated in multiple collisions and undergo isomerization and fragmentation. U_{tr} from top to bottom: 10 V, 20 V, and 40 V. The ratios of the fast and slow components are: U_{tr} = 10 V: 10:2; U_{tr} = 20 V: 10:7; U_{tr} = 40 V: 2:10.

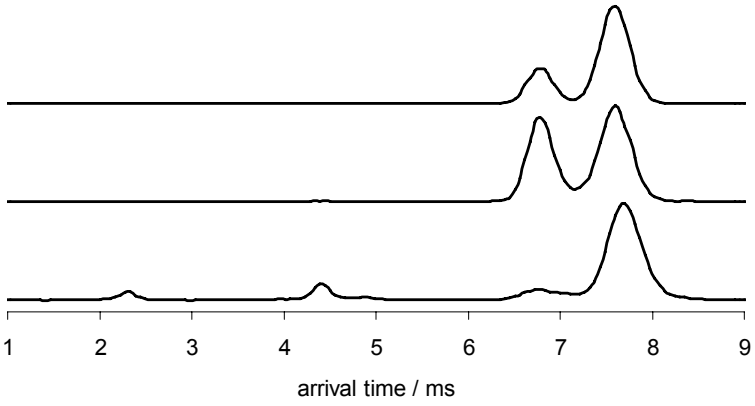


Figure S15. Ion-mobility traces of the mass-selected protonated ion *anti*-**2**H^+ (*m/z* 467) at different voltages (U_{tr}) applied to the ion trap in front of the ion-mobility device. U_{tr} from top to bottom: 10 V, 20 V, and 40 V. The ratios of the fast and slow components are: U_{tr} = 10 V: 3:10; U_{tr} = 20 V: 7:10; U_{tr} = 40 V: 1:10.

Collision-induced fragmentation of $2H^+$ in the transfer cell after the IM unit

A mixture of *syn*-**2** and *anti*-**2** was investigated by collision-induced dissociation in the transfer cell behind the ion-mobility section (Figure S16). The observed fragmentation patterns are identical for both diastereoisomers, but the total amount of fragmentation is slightly smaller for *anti*-$\mathbf{2}H^+$ (56.6 ± 0.8 %) than for *syn*-$\mathbf{2}H^+$ (58.1 ± 0.7 %) implying that that *anti*-$\mathbf{2}H^+$ is slightly more stable than the *syn* isomer.

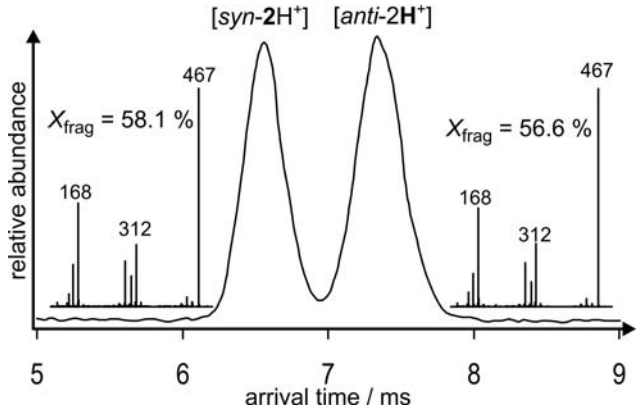


Figure S16. Ion-mobility trace of the mass-selected protonated ions $\mathbf{2}H^+$ (m/z 467) generated from a ca. 1:1 mixture of *syn*-**2** and *anti*-**2** under soft ionization conditions (U_c = 20 V) and the collision-induced dissociation mass spectra of the fast and the slow components.

Collisional activation of $2Na^+$ and $2Ag^+$ species

Figure S17 shows the ion-mobility traces for mass-selected *syn*-**2**Na^+ as well as for *anti*-**2**Na^+ generated at different cone voltages in the ESI source. Contrary to the protonated species, the ion-mobility traces of sodiated species have only one peak (at 5.8 ms for *syn*-**2**Na^+ and at 7.3 ms for *anti*-**2**Na^+) even at elevated cone voltages. Thus, **2**Na^+ does not undergo epimerization.

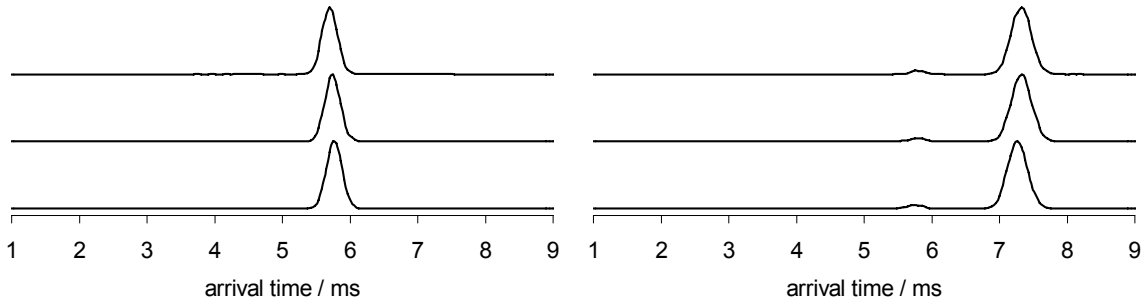


Figure S17. Ion-mobility traces of the mass-selected sodiated ions (*m/z* 489) for *syn*-**2** (left) and *anti*-**2** (right) at different cone voltages (U_c) in the ESI source. U_c from top to bottom: 20 V, 40 V, and 60 V.

Figure S18 depicts the ion-mobility traces of mass-selected *syn*-**2**Na^+ and *anti*-**2**Na^+ at several applied trap voltages. It can be seen, that **2**Na^+ species do not show either epimerization or fragmentation upon collisional activation in the ion trap. The intensity of *anti*-**2**Na^+ was already too low at 30 V therefore recording spectrum at that voltage was impossible.

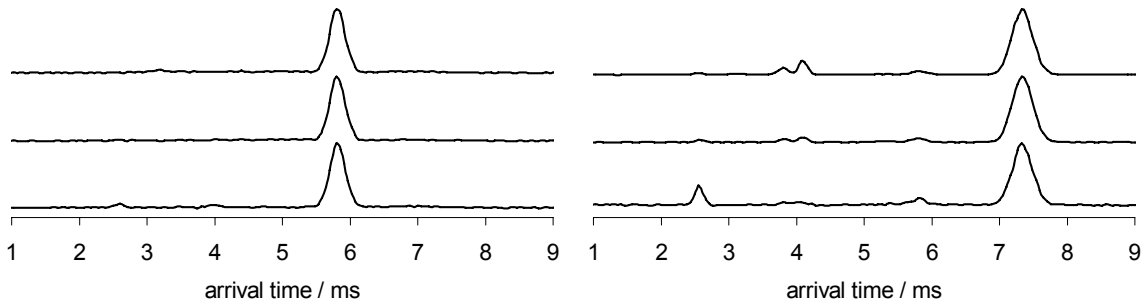


Figure S18. Ion-mobility traces of the mass-selected sodiated ions (*m/z* 489) for *syn*-**2** (left) and *anti*-**2** (right) at different cone voltages (U_{tr}) applied to the ion trap in front of the mobility cell. U_{tr} from top to bottom: 10 V, 20 V, 30 V and 10 V, 20V, 25 V in case of *syn*-**2** and *anti*-**2**, respectively.

The ion-mobility traces of ca. 1:1 mixture of *syn*-**2** and *anti*-**2** for the mass-selected sodiated ions (**2**Na^+) was recorded at different voltages applied in the ion trap. As it can be seen in Figure S19 the ratio of the areas of the fast (early) and slow (late) components changes with the applied voltage. The larger U_{tr}, the bigger the fractional abundance of early (*syn*-**2**Na^+) component despite the fact that isomerization does not takes place. This result implies that the binding energy of Na^+ is larger in *syn*-**2**Na^+ than in *anti*-**2**Na^+ and the ratio of the two component changes because the decrease of

the amount of *anti*-**2**Na^+ by loss of Na^+ (the resulting bare Na^+ fragment ion is out of the mass range of the SYNAPT G2 and therefore cannot be detected). Since, the energy of the two isomers of neutral compound **2** are very close in energy (see full text), the binding energy difference implies that the *syn*-**2**Na^+ is more stable than *anti*-**2**Na^+.

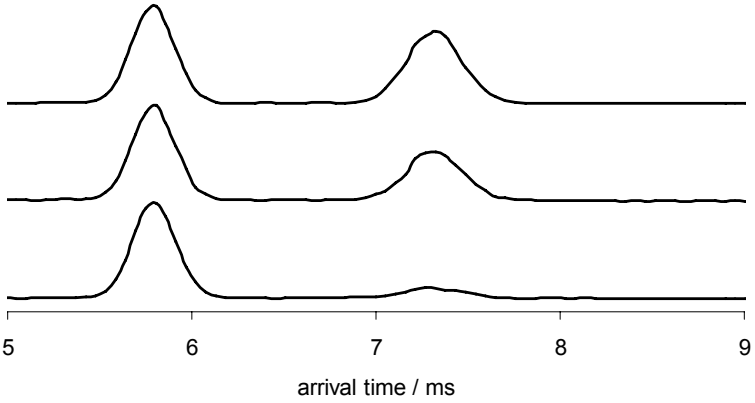


Figure S19. Ion-mobility traces of the mass-selected sodiated ions **2**Na^+ (*m/z* 489) at different voltages (U_{tr}) applied to the ion trap. U_{tr} from top to bottom: 10 V, 20 V, and 30 V.

The argentated species were investigated analogously to the sodiated species and behaved similarly. Figure S20 and Figure S21 show the ion-mobility traces for mass-selected *syn*-**2**Ag^+ as well as for *anti*-**2**Ag^+ at different voltages applied in the ESI source and to the ion trap in front of the ion-mobility device, respectively. Similarly to the sodiated species, the argentated ions have only one component (at 6.1 ms for *syn*-**2**Ag^+ and at 7.0 ms for *anti*-**2**Ag^+) even at elevated voltages. Thus, just like **1**Ag^+, **2**Ag^+ does not undergo epimerization. The fast component at 4.6 ms in the IM-MS trace of *anti*-**2**Ag^+ at low voltage again comes from the dimmer. The peak at 7.3 ms appearing at large trap voltage is due to AgH loss.

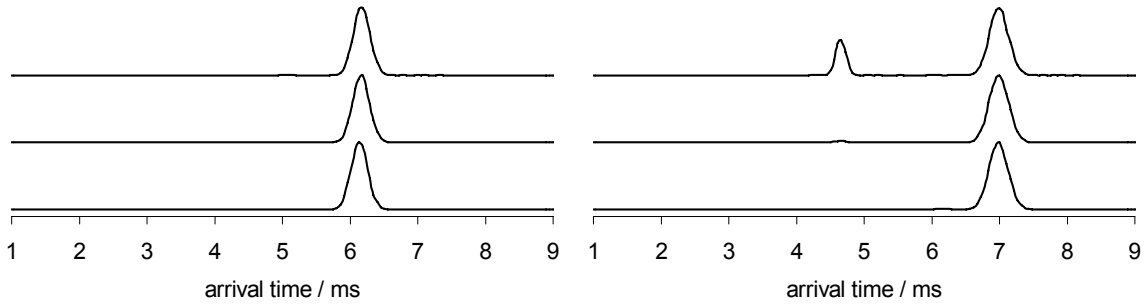


Figure S20. Ion-mobility traces of the mass-selected argentated ions (*m/z* 573) for *syn*-**2** (left) and *anti*-**2** (right) recorded at different cone voltages (U_c). U_c from top to bottom: 20 V, 40 V and 60 V.

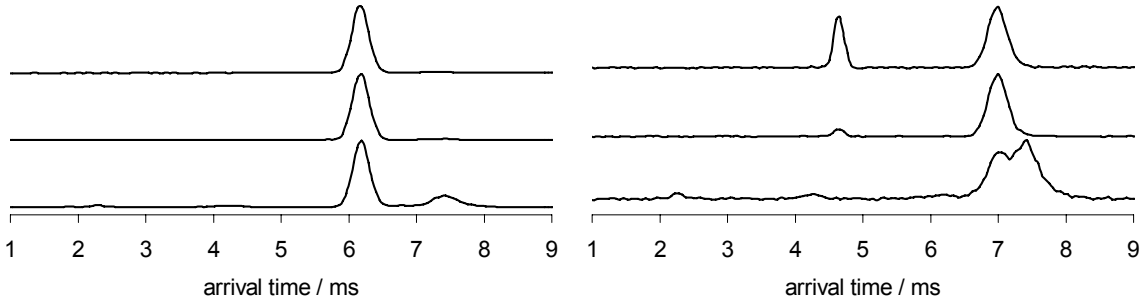


Figure S21. Ion-mobility traces of the mass-selected argentated ions (*m/z* 573) for *syn*-**2** (left) and *anti*-**2** (right) recorded at different voltages applied to the trap (U_{tr}). U_{tr} from top to bottom: 10 V, 20 V and 40 V. The larger amount of AgH loss in case of anti (see component at 7.3 ms) indicates the bigger stability of the *syn* isomer.

The ion-mobility measurement of mixture of *syn*-**2** and *anti*-**2** was repeated for the mass-selected argentated ions (**2**Ag^+) at different voltages applied in the ion trap. Similarly to the sodium complexes the ratio of the areas of the fast and slow components changes with the applied voltage. The larger U_{tr}, the bigger the fractional abundance of early (*syn*-**2**Ag^+) component although epimerization does not takes place (Figure S22). The ratio of the two components changes because the decrease of the amount of *anti*-**2**Ag^+ by loss of AgH giving the new component at 7.3 ms.

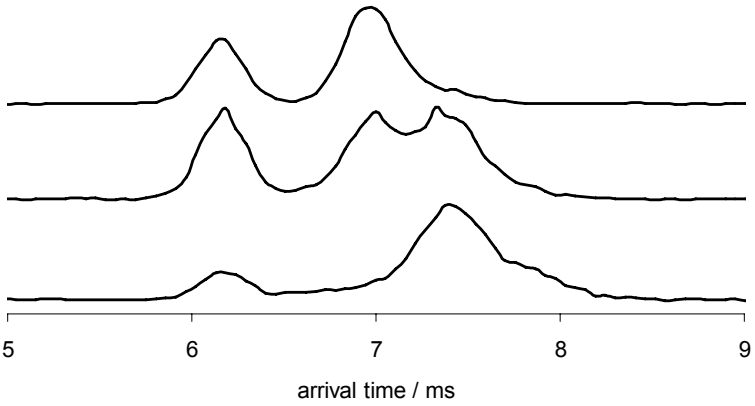


Figure S22. Ion-mobility traces of the mass-selected argentated ions **2**Ag^+ (*m/z* 573) at different voltages (U_{tr}) applied to the ion trap. U_{tr} from top to bottom: 30 V, 40 V, and 50 V.

Additional MS and MS/MS spectra proving the existence of the dimer (*anti*-2Ag)$_2^{2+}$

The mass spectrum and the associated ion mobility traces of the peaks having different *m/z* values are shown in Figure S23 and Figure S24 for *syn*-**2** and *anti*-**2** in the presence of Ag^+, respectively. In the *anti* case, the mass spectrum has peaks at half masses and the ion-mobility traces show two components. In contrast, the *syn* case shows only peaks at whole masses in the MS and the corresponding ion-mobility traces are one-component.

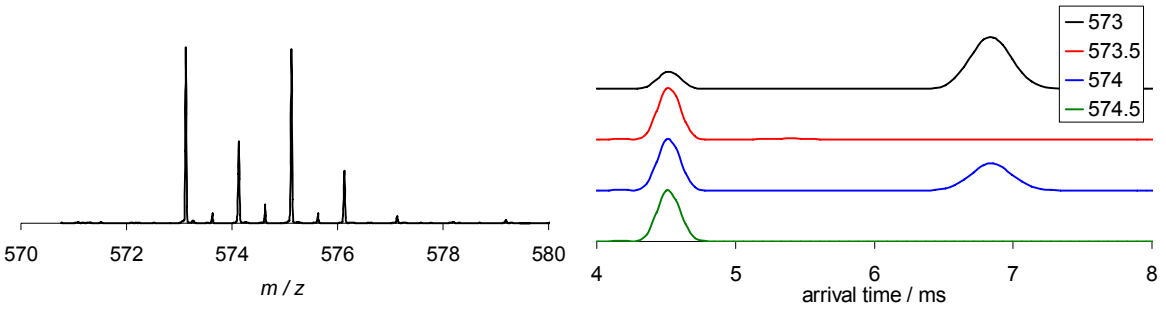


Figure S23. Overview mass spectrum around *m/z* 573 (left) and the corresponding ion-mobility traces of the peaks having different *m/z* values (right) for a solution of *anti*-**2** (*c* = $1.1 \cdot 10^{-5}$ M) with added $AgNO_2$ (c = $6.2 \cdot 10^{-5}$ M).

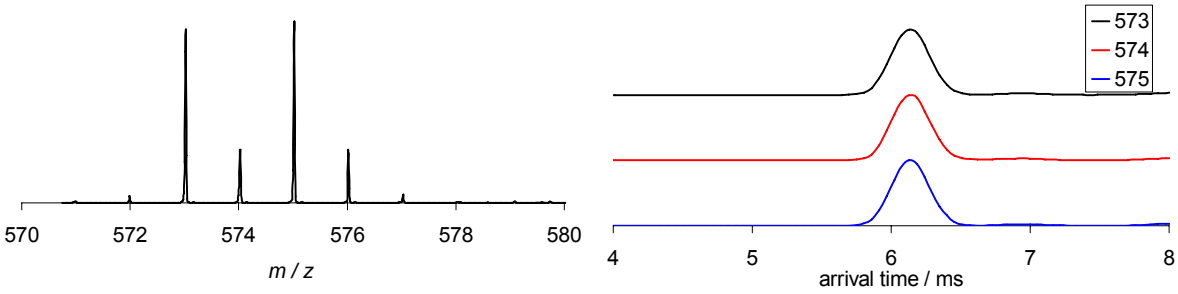


Figure S24. Overview mass spectrum around *m/z* 573 (left) and the corresponding ion-mobility traces of the peaks having different *m/z* values (right) for a solution of *syn*-**2** (*c* = $1.1 \cdot 10^{-5}$ M) with added $AgNO_2$ (c = $6.2 \cdot 10^{-5}$ M).

Figure S25 shows the mass spectra of the mass-selected ^{13}C-(*anti*-**2**Ag)$_2^{2+}$ at *m/z* 573.5 at different ion trap voltages applied in front of the mobility cell as well as the associated ion-mobility traces. At low voltage, the mass spectrum has one major peak at *m/z* 537.5 and two minor ones at *m/z* 573 and 574, while the mobility trace shows one major component at around 4.6 ms with a small contribution at ca. 7.0 ms. Upon excitation, the relative intensity of fragment peaks at *m/z* 573 and 574 increases which is associated with the increase of the component at 7.0 ms in the mobility traces. These results are in agreement with the dissociation of the dimer into monomers having *m/z* 573 and 574.

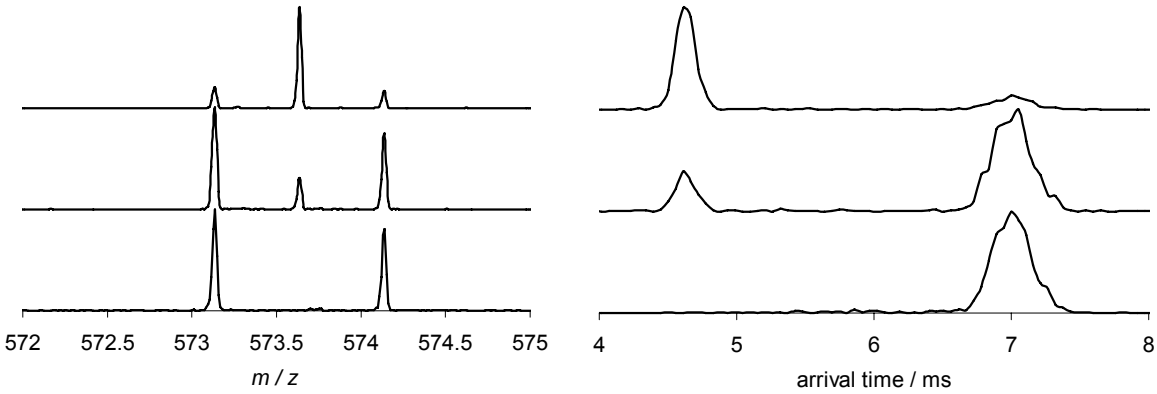


Figure S25. Mass spectra and the associated ion-mobility traces of the mass-selected ^{13}C-(anti-2Ag)$_2^{2+}$ (m/z 573.5) at different voltages (U_{tr}) applied to the ion trap. U_{tr} from top to bottom: 10 V, 20 V, and 30 V.

Collision-induced isomerization of $3H^+$ in the trap prior to the IM unit

The investigation of the effect of the voltage applied to the ion trap was performed with mass-selected *syn,syn*-**3**H^+, *syn,anti*-**3**H^+ and *anti,anti*-**3**H^+. The findings are in agreement with those for activation by cone voltage in the ESI source (see Figure 7 in the full text): isomerisation to the other isomers and fragmentation take place at elevated voltages.

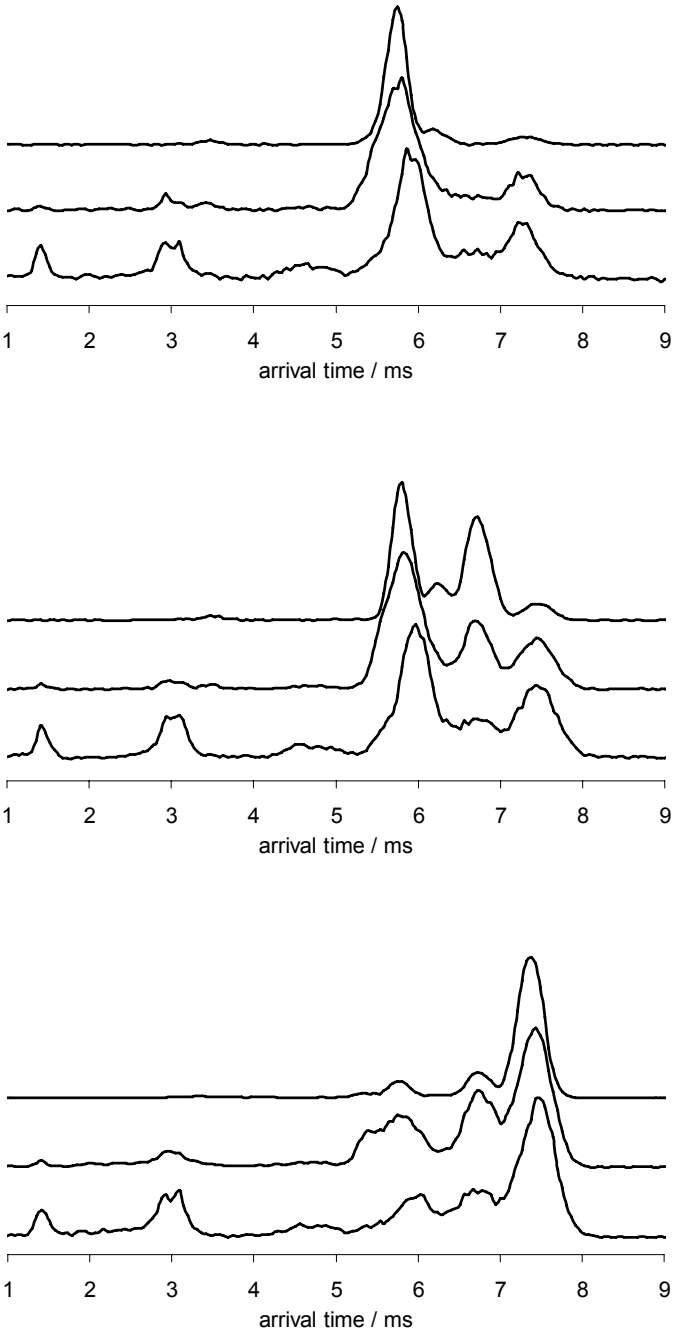


Figure S26. Ion-mobility traces of the mass-selected protonated ion **3**H^+ (*m/z* 611) for *syn,syn*-**3** (top), *syn,anti*-**3** (middle) and *anti,anti*-**3** (bottom) at different voltages (U_{tr}) applied to the ion trap in front of the ion-mobility device. U_{tr} from top to bottom: 10 V, 30 V, and 40 V.

Collision-induced fragmentation of $3H^+$ in the transfer cell after the IM unit

A mixture of *syn,syn*-**3,** *syn,anti*-**3** and *anti,anti*-**3** was investigated by collision-induced dissociation in the transfer cell behind the ion-mobility section (Figure S27). The observed fragment ions are same for all isomers, but their relative intensities as well as the total amount of fragmentation is slightly different.

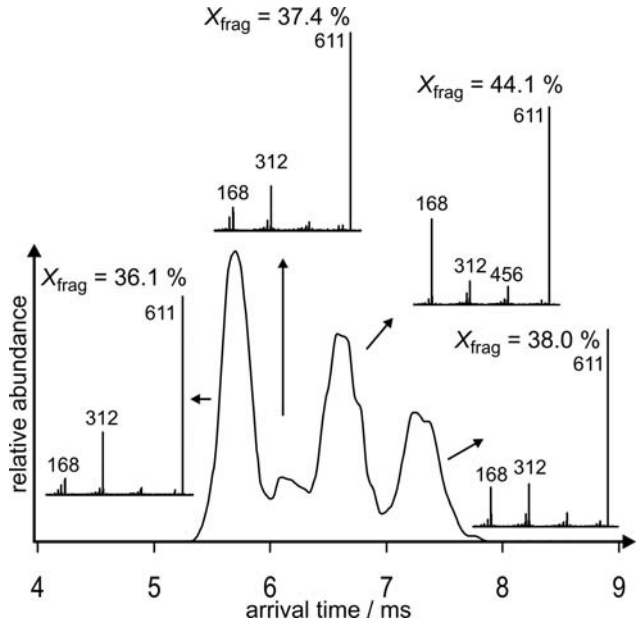


Figure S27. Ion-mobility trace of the mass-selected protonated ions **3**H^+ (m/z 611) generated from a mixture of *syn,syn*-**3,** *syn,anti*-**3** and *anti,anti*-**3** and the collision-induced dissociation mass spectra of the three isomers as well as that of the peak appearing at ca. 6.1 ms.

Collisional activation of $3Na^+$ and $3Ag^+$ species

Figure S28 shows the ion-mobility traces for mass-selected *syn,syn*-**3**Na^+, *syn,anti*-**3**Na^+ and *anti,anti*-**3**Na^+ generated at different cone voltages in the ESI source. Similarly to the case of bis-TBs **1** and **2**, the ion-mobility traces of sodiated species have mainly only one peak (at 5.4 ms for *syn,syn*-**3**Na^+, at 6.0 ms for *syn,anti*-**3**Na^+ and at 7.2 ms for *anti,anti*-**3**Na^+) even at elevated cone voltages, and the **3**Na^+ species do not undergo isomerization.

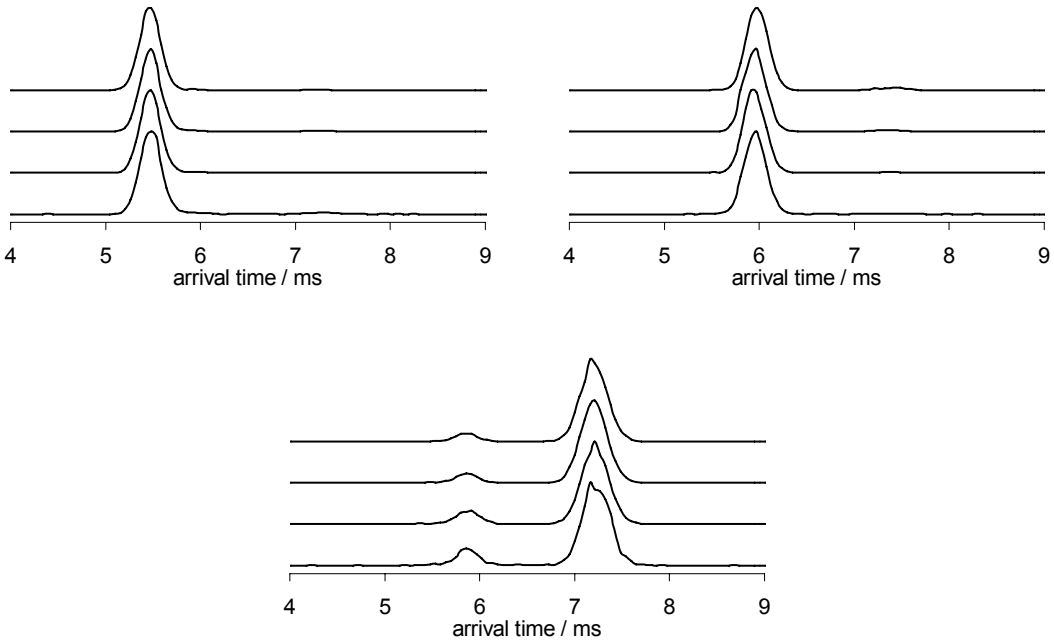
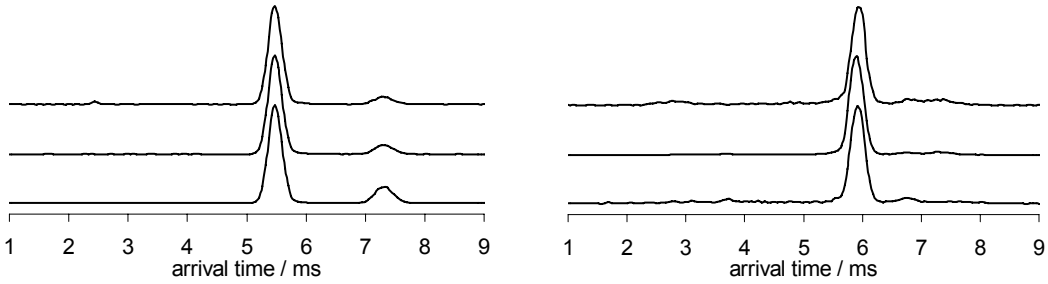


Figure S28. Ion-mobility traces of the mass-selected sodiated ions (*m/z* 633) for *syn,syn*-**3** (top, left) *syn,anti*-**3** (top, right) and *anti,anti*-**3** (bottom) at different cone voltages (U_c) in the ESI source. U_c from top to bottom: 40 V, 60 V, 80 V and 100 V.

Figure S29 depicts the ion-mobility traces of mass-selected *syn,syn*-**3**Na^+, *syn,anti*-**3**Na^+ and *anti,anti*-**3**Na^+ at several trap voltages applied to the ion trap in front of the mobility section. Just like **2**Na^+ ions, **3**Na^+ species do not undergo either isomerization or fragmentation upon collisional activation. The intensity of *anti,anti*-**3**Na^+ was already too low at 30 V therefore the highest voltage at which spectrum was recorded is 25 V.



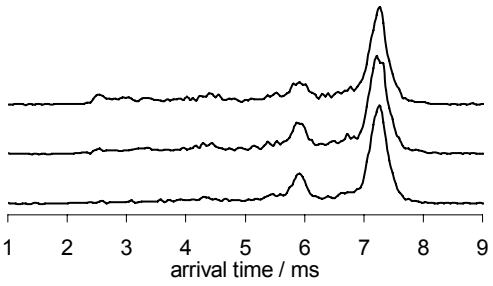


Figure S29. Ion-mobility traces of the mass-selected sodiated ions (*m/z* 633) for *syn,syn*-**3** (top, left) *syn,anti*-**3** (top, right) and *anti,anti*-**3** (bottom) at different trap voltages (U_{tr}). U_{tr} from top to bottom: 10 V, 30 V and 40 V in case of *syn,syn* and *syn,anti* isomer and 10 V, 20 V and 25 V for *anti,anti* isomer, respectively.

The ion-mobility traces of ca. 1:1:1 mixture of *syn,syn*-**3**, *syn,anti*-**3** and *anti,anti*-**3** for the mass-selected sodiated ions (**3**Na^+) were recorded at different voltages applied in the ion trap. Figure S30 depicts the obtained spectra. Upon excitation, the relative abundance of the slowest component decreases. Since epimerization does not take place, this implies that *anti,anti*-**3**Na^+ is less stable than *syn,anti*-**3**Na^+ and *syn,syn*-**3**Na^+. This can be explained by the cage structure of the latter two isomers.

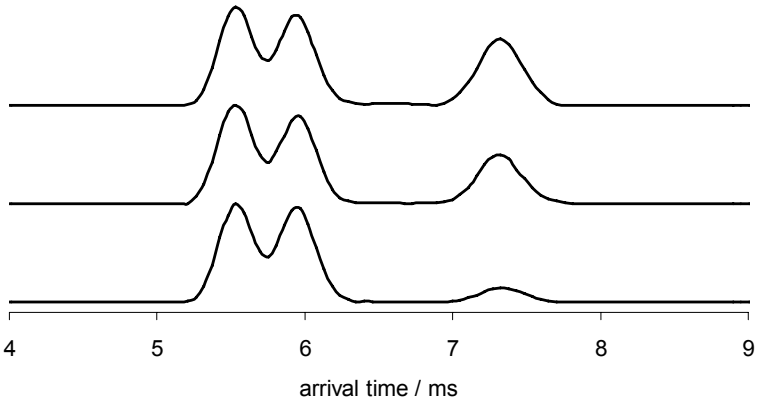


Figure S30. Ion-mobility traces of the mass-selected sodiated ions **3**Na^+ (*m/z* 633) at different voltages (U_{tr}) applied to the ion trap. U_{tr} from top to bottom: 8 V, 25 V and 35 V.

The argentated species were investigated analogously to the sodiated species and behaved similarly. Figure S31 and Figure S32 show the ion-mobility traces for mass-selected *syn,syn*-**3**Ag^+, *syn,anti*-**3**Ag^+ and *anti,anti*-**3**Ag^+ at different voltages applied in the ESI source and to the ion trap in front of the ion-mobility separation, respectively. Similarly to the sodiated species, the argentated ions have only one component (at 5.4 ms for *syn,syn*-**3**Ag^+, at 6.2 ms for *syn,anti*-**3**Ag^+ and at 7.1 ms for *anti,anti*-**3**Ag^+) even at elevated voltages. Thus, just like **1**Ag^+ and **2**Ag^+, **3**Ag^+ does not undergo epimerization. The fast component at 4.1 ms in the IM-MS trace of *anti,anti*-**3**Ag^+ at low voltage

most likely comes from a dimer, analogously to *anti*-**2**Ag^+. The AgH loss appears at ca. 7.2 ms and therefore is not baseline separated from the *anti,anti*-**3**Ag^+.

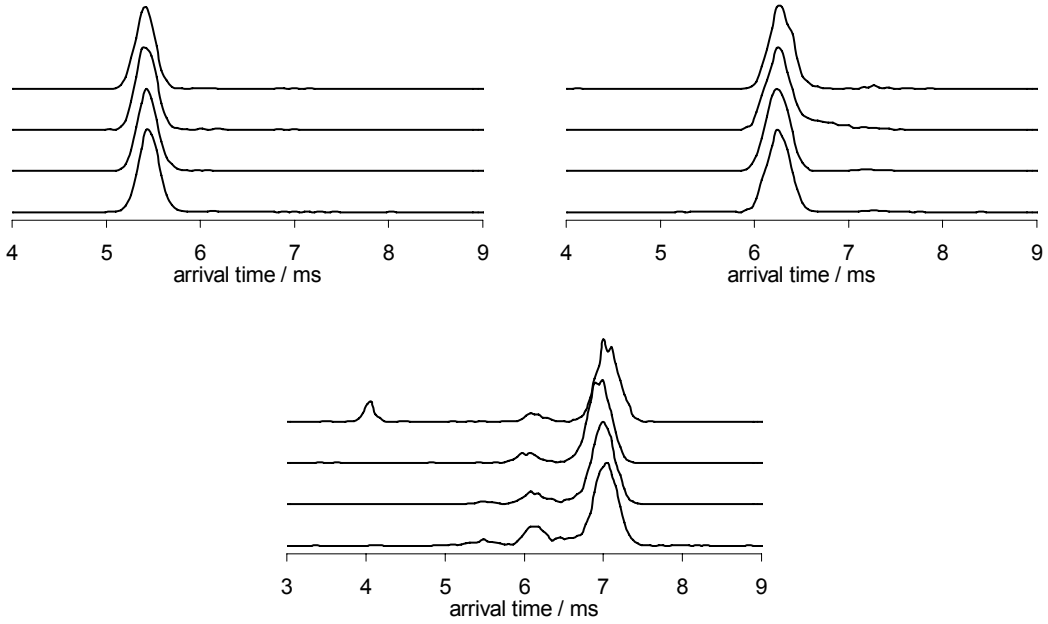


Figure S31. Ion-mobility traces of the mass-selected argentated ions (*m/z* 717) for *syn,syn*-**3** (top, left) *syn,anti*-**3** (top, right) and *anti,anti*-**3** (bottom) at different cone voltages (U_c) in the ESI source. U_c from top to bottom: 40 V, 60 V, 80 V and 100 V.

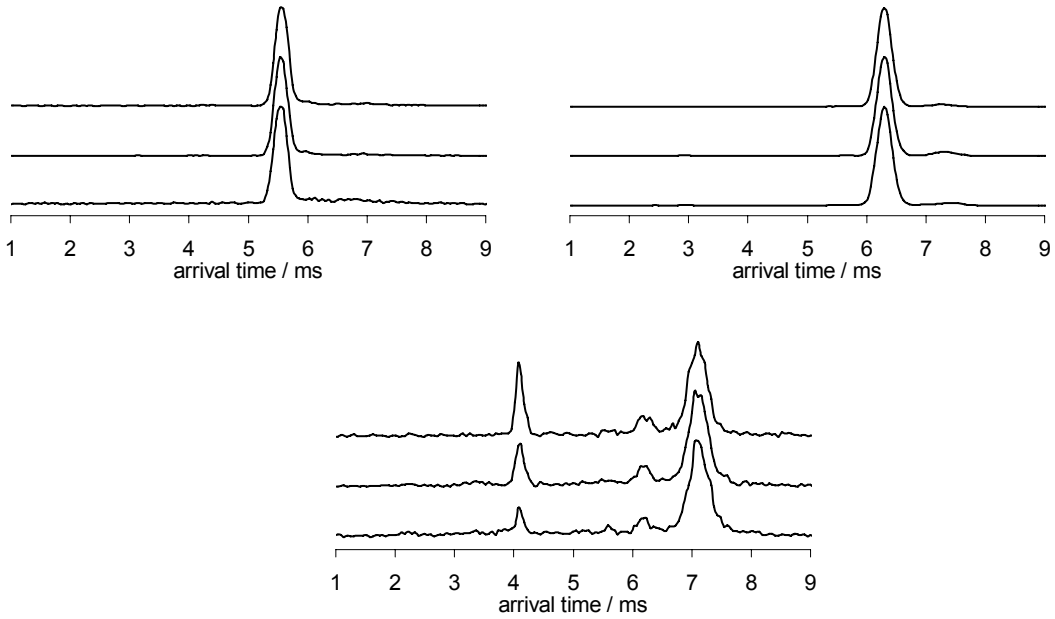


Figure S32. Ion-mobility traces of the mass-selected argentated ions (*m/z* 717) for *syn,syn*-**3** (top, left) *syn,anti*-**3** (top, right) and *anti,anti*-**3** (bottom) at different trap voltages (U_{tr}). U_{tr} from top to bottom: 10 V, 30 V and 40 V in case of *syn,syn* and *syn,anti* isomer and 10 V, 20 V and 25 V for *anti,anti* isomer, respectively.

The ion-mobility traces of a mixture of *syn,syn*-**3**, *syn,anti*-**3** and *anti,anti*-**3** for the mass-selected argentated ions (**3**Ag^+) at different voltages applied to the trap are depicted in Figure S33. Upon excitation, the relative abundance of the slowest component decreases showing that *anti,anti*-**3**Ag^+ is less stable than *syn,anti*-**3**Ag^+ and *syn,syn*-**3**Ag^+. This can be explained by the cage structure of the latter two isomers.

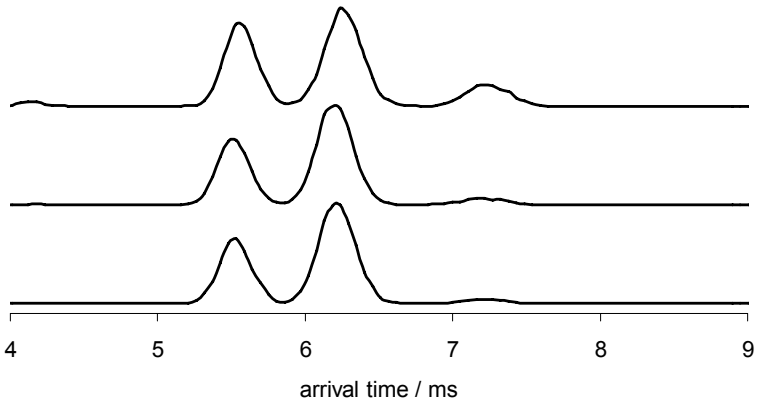


Figure S33. Ion-mobility traces of the mass-selected argentated ions **3**Ag^+ (*m/z* 717) at different voltages (U_{tr}) applied to the ion trap. U_{tr} from top to bottom: 10 V, 20 V and 30 V.

Calculated structures of the (*anti*-2Ag)$_2^{2+}$ dimer and comparison of cross section to experiments

Several computations were run to identify the trends governing the stability of various forms of the dicationic dimer complex. Structural, energetic, and cross section data for some isomers are shown in Table S1 and Figure S34 below; the ones mentioned in the paper are denoted by **d1** and **d2**. We found that in general, complexes held together only by noncovalent interactions (**d3**) exist as local minima, but they lie at higher energies than two molecules of *anti*-**2**Ag$^+$ despite the fact that they maximize the distance between the silver cations. Apparently, the silver ions prefer coordination to the nitrogen, even if this means that they get somewhat closer to each other (**d2,d4,d5**). On the other hand, coordination of one of them simultaneously to two nitrogen atoms cannot balance the effect of the stronger repulsion in the resulting Ag$^+$–N–CH$_2$–N–Ag$^+$ fragment (**d6**). Hence, there seems to be a preference for the *N*,π coordination with the two involved nitrogens coming from different molecules, but the silver ions must still be attached to more distinct organic parts, otherwise, their repulsion will be too high (**d7**,**d8**). The most stable structures are therefore **d1** and **d2**.

To investigate the experimental ion-mobility results on the dimers, we first determined the exponential factor *x* using the results for the monomers only (all complexes of **2** and **3**, 15 points altogether), obtaining 0.5436. The resulting corrected arrival times, together with the linear fit to the monomer values, are shown in Figure S35, where the cross section values for all computed isomers of the dimer are also depicted. As apparent, all isomers fall rather close to the line, only **d7** is somewhat farther away. While we cannot resolve very fine structural details on the basis of hard-sphere cross section calculations, particularly when the unknown isomers are far off the range of known data points, the good fit of the supposed dimer structures is encouraging.

Table S1. Composition, cross section, and energy of various isomers of (*anti*-**2**Ag)$_2^{2+}$

Isomer	Composition[a]	Cross section (Å^2)	Relative energy[b] (kJ/mol)
d1	**+−**	267.79	**-53.64**
d2	**++**	275.46	**-44.76**
d3	**+−**	279.26	**60.44**
d4	**++**	266.12	**-29.00**
d5	**++**	267.91	**-13.22**
d6	**++**	291.05	**17.89**
d7	**++**	254.28	**-3.43**
d8	**++**	273.57	**-5.73**

[a] Dimers contain two identical (+ +) or mirror image (+ −) copies of *anti*-**2**.
[b] Relative to two molecules of *anti*-**2**Ag$^+$

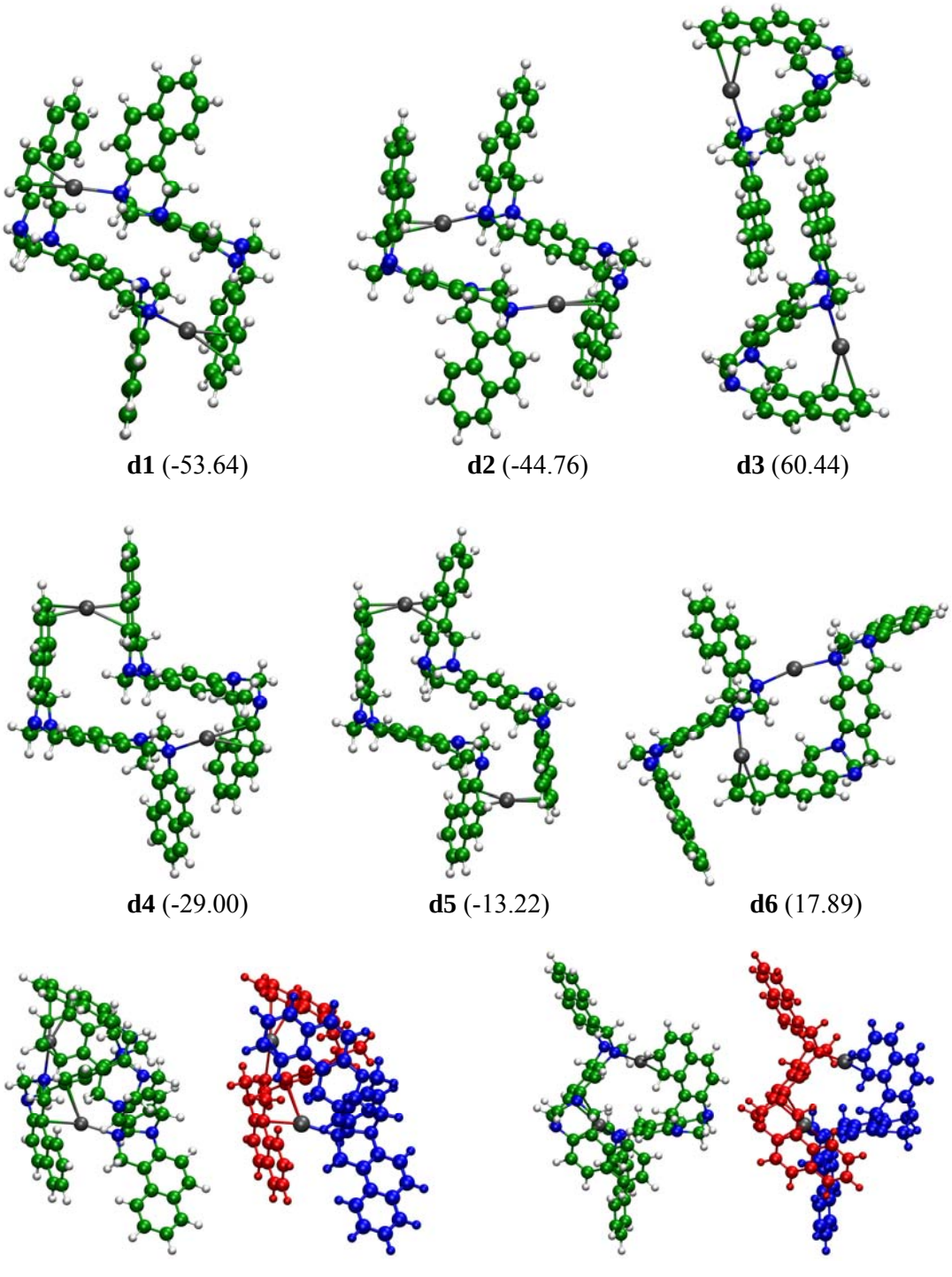


Figure S34. Structures and relative energies (kJ/mol, with respect to 2 molecules of *anti*-**2**Ag^{+}) of isomers of (*anti*-**2**$Ag)_2^{2+}$.

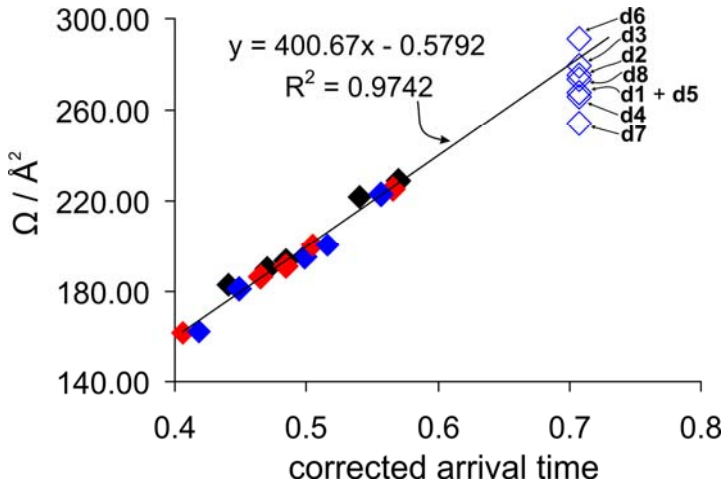
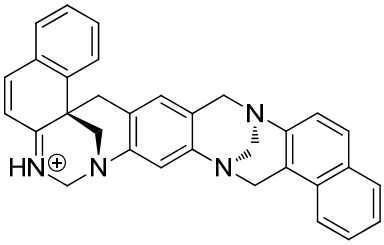
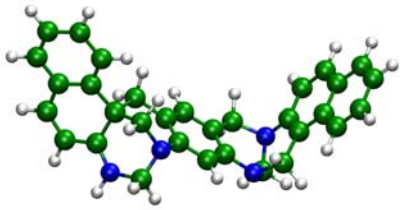


Figure S35. Corrected arrival times (with x = 0.5436) and computed cross sections for monomer structures of complexes of **2** and **3** (unlabeled, filled diamonds) and for the dimer candidates (labeled, empty diamonds) of $(anti\text{-}\mathbf{2}Ag)_2^{2+}$. Black: protonated species, red: Na^+ complexes, blue: Ag^+ complexes. The linear fit was obtained using the monomers.

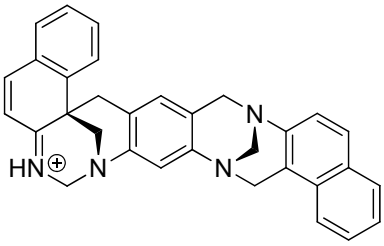
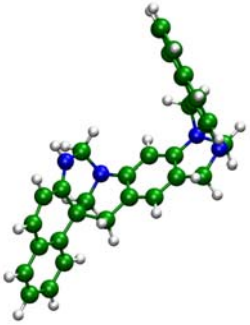
Spiro isomers of bis-TB 2 and tris-TB 3

As mentioned in the main text of the paper, we hypothesize that protonated TBs might undergo other isomerization processes besides pseudo-epimerization. Scission of the N–C bond between the benzylic CH_2 and the protonated nitrogen can lead to the conversion of the TB framework to the spiro-TB structure. The price to be paid is the loss of the aromaticity in one of the rings; this will be the ring that is directly connected to the originally protonated nitrogen. The computations revealed that there are only minor differences among the stabilities of the normal TB isomers protonated at different positions, thus formation of any spiro-TB is in principle conceivable. As apparent from Figure S36, for the bis-TB **2**, spiro(out) isomers, with one ring of the naphthalene moiety attacked (keeping the other half aromatic), are notably more stable than spiro(in) isomers, with the benzene ring losing aromaticity, in agreement with expectations on the basis of the resonance energies. For this reason, only naphthalene-attacked isomers were investigated for the tris-TB **3**; the identified isomers are shown in Figure S37. The surprising stability of the *syn*,*syn* spiro structure can probably be explained by the fact that in this isomer, the N–H bond of the protonated iminium moiety can form an intramolecular N–H···π type hydrogen bond with the naphthalene ring at the other end of the molecule. We note that such an arrangement could not be realized in spiro-**3**H^+ isomers with the benzene ring attacked. While the *syn*,*syn*-spiro isomer is even more stable in the gas phase than any normal one, the barrier for spiro formation is probably higher than that of the pseudo-epimerization because in the latter process, no rings lose aromaticity upon breaking the N–C bond. This suggests that the spiro isomers should only be observable at most in small quantities, in accordance with the solution phase results where this conversion was not observed.

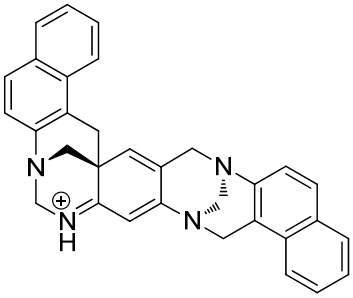
Using the linear correlation shown in Figure 9 of the paper and the further parameters, such as the exponential factor *x*, we can predict the experimentally observable, uncorrected arrival times of the computed spiro structures. The numbers are shown in Figures S36 and S37, and in Figure S38, they are depicted for comparison with the experimentally observed mobility traces for **2**H^+ and **3**H^+. It is clear that the spiro isomers fall into the range where the larger peaks and the small additional ones are observed experimentally, but once again, the error of the modeling does not allow to draw firm conclusions about structural details in a large set of similarly-shaped isomers.

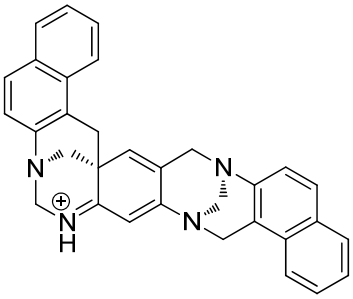
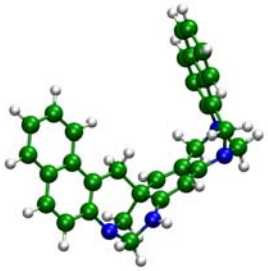
anti-spiro(out)-**2**H$^+$ 7.40 kJ mol^{-1} 189.26 Å^2 5.14 ms

syn-spiro(out)-**2**H$^+$ 6.71 kJ mol^{-1} 187.16 Å^2 5.03 ms




anti-spiro(in)-**2**H$^+$ 19.49 kJ mol^{-1} 189.13 Å^2 5.13 ms

syn-spiro(in)-**2**H$^+$ 22.50 kJ mol^{-1} 182.25 Å^2 4.79 ms

Figure S36. Spiro-**2**H$^+$ isomers. The numbers are the computed relative stabilities with respect to *anti*-**2**H$^+$, the calculated hard-sphere cross sections, and the estimated uncorrected arrival times.

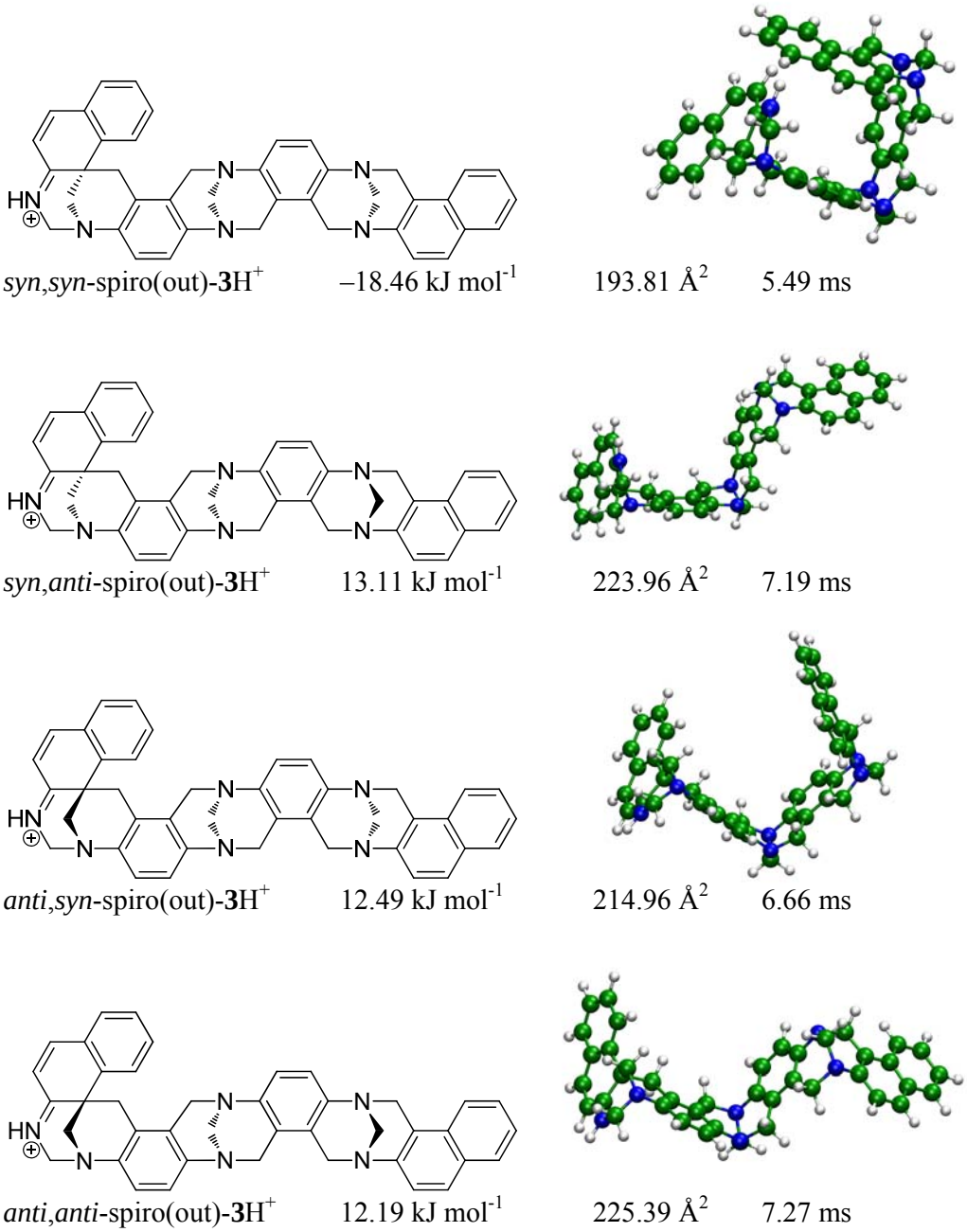


Figure S37. Spiro-**3**H$^+$ isomers. The numbers are the computed relative stabilities with respect to *anti*,*anti*-**3**H$^+$, the calculated hard-sphere cross sections, and the estimated uncorrected arrival times.

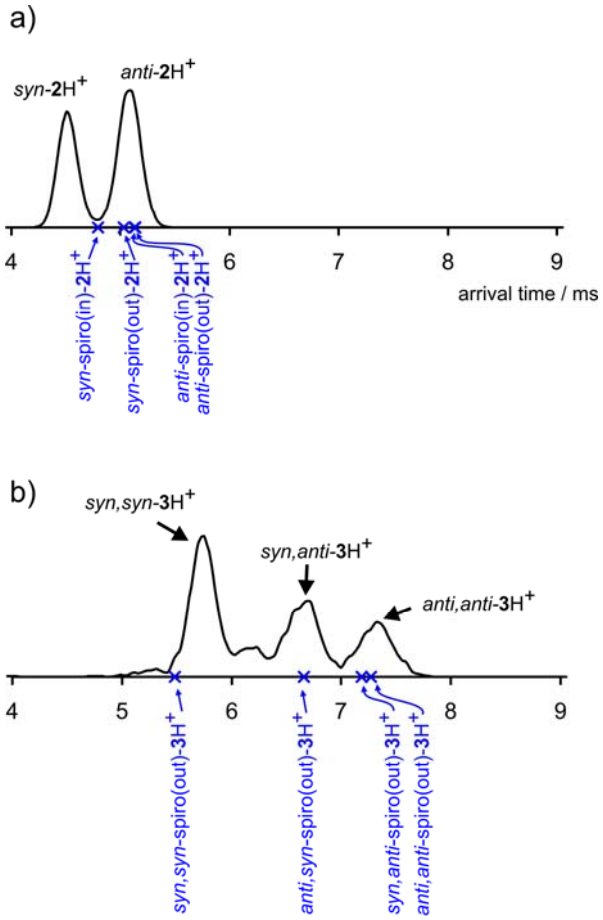


Figure S38. Experimental ion mobility traces (black lines) for isomer mixtures of **2**H^+ (a) and **3**H^+ (b) (both measured with the parameters used in the study of **3**), together with the computed (uncorrected) arrival times for the investigated spiro isomers (blue crosses on the axis).

Relative energies, structures, and cross sections of derivatives of bis-TB 2

Table S2. Computed cross sections and relative energies for all considered isomers of complexes of bis-TB **2.** Dimer structures of *anti*-**2**Ag^+ are discussed in a separate section of the Supporting Information and not included here.

Structure	Cross section ($Å^2$)	Relative energy[a]
syn-**2**	181.79	**0.06**
syn-**2**H^+–in	182.75	**-961.08**
syn-**2**H^+–out	182.32	**-958.17**
syn-**2**Na^+	161.93	**-209.84**
syn-**2**Ag^+	162.44	**-323.11**
anti-**2**	189.77	**0.00**
anti-**2**H^+–in	190.28	**-961.13**
anti-**2**H^+–out	190.38	**-958.38**
anti-**2**Na^+–π	186.74	**-176.81**
anti-**2**Na^+–N	183.08	**-159.89**
anti-**2**Ag^+	180.94	**-281.18**
anti-spiro(in)-**2**H^+	189.13	**-941.63**
syn-spiro(in)-**2**H^+	182.25	**-938.63**
anti-spiro(out)-**2**H^+	189.26	**-953.73**
syn-spiro(out)-**2**H^+	187.16	**-954.41**

[a] Energies are relative to *anti*-**2** plus the corresponding cation (H^+, Na^+, Ag^+) if necessary.

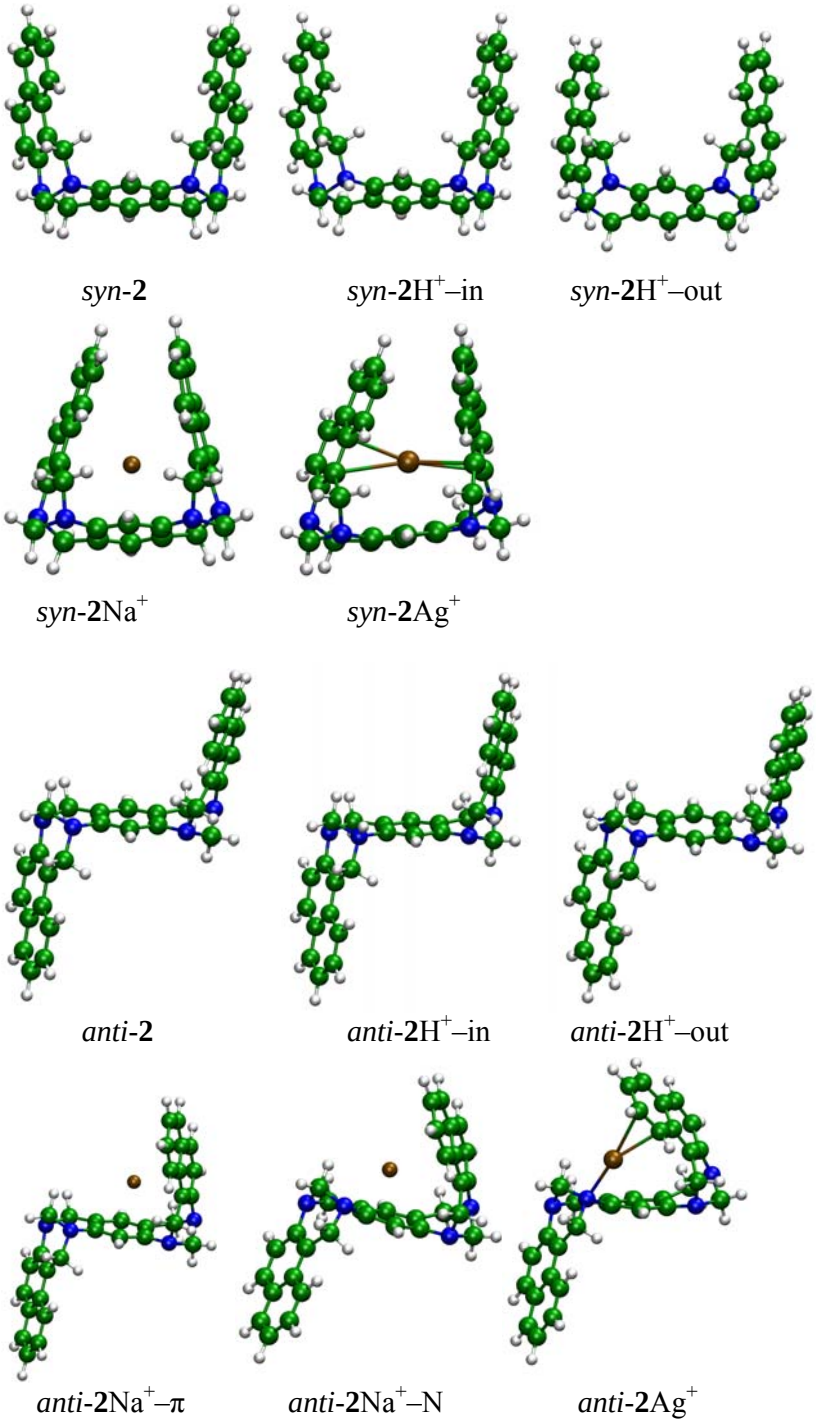


Figure S39. Various structures for derivatives of **2**. Dimer structures of *anti*-**2**Ag$^+$ and spiro isomers of **2**H$^+$ are shown in a separate section of the Supporting Information.

Relative energies, structures, and cross sections of derivatives of tris-TB 3

Table S3. Computed cross sections and relative energies for all considered isomers of complexes of tris-TB **3**. The place where the cationizing species (H^+, Na^+, Ag^+) binds is denoted using numbers for the nitrogen atoms, uppercase letters for rings, and lowercase letters for individual π-bonds (see Figure S40). Marked in red are the most stable geometries of a certain cationized version of a certain diastereomer (e.g., the most stable among all *syn,syn*-**3**H^+ variations)

Structure	Cross section (Å^2)	Relative energy[a]
syn,*syn*-**3**	194.63	**0.77**
syn,*syn*-**3**H^+–1	194.21	**-958.56**
syn,*syn*-**3**H^+–2	194.25	**-963.83**
syn,*syn*-**3**H^+–3	195.38	**-964.49**
syn,*syn*-**3**Na^+–AA'	193.50	**-216.80**
syn,*syn*-**3**Na^+–ABB'	190.61	**-214.86**
syn,*syn*-**3**Ag^+–AiB'f	191.26	**-326.53**
syn,*syn*-**3**Ag^+–AkA'g	193.07	**-310.45**
syn,*syn*-**3**Ag^+–AiB'a	192.31	**-326.21**
syn,*anti*-**3**	221.24	**1.06**
syn,*anti*-**3**H^+–1	221.87	**-955.48**
syn,*anti*-**3**H^+–2	221.86	**-961.36**
syn,*anti*-**3**H^+–3	221.46	**-964.13**
syn,*anti*-**3**H^+–3'	221.60	**-964.24**
syn,*anti*-**3**H^+–2'	220.57	**-963.26**
syn,*anti*-**3**H^+–1'	221.08	**-956.86**
syn,*anti*-**3**Na^+–ABB'	200.69	**-221.19**
syn,*anti*-**3**Na^+–A'B'	218.48	**-175.37**
syn,*anti*-**3**Ag^+–AaB'c	200.43	**-333.36**
syn,*anti*-**3**Ag^+–Af2'	205.96	**-330.21**
anti,*anti*-**3**	228.35	**0.00**
anti,*anti*-**3**H^+–1	228.92	**-956.71**
anti,*anti*-**3**H^+–2	228.82	**-962.67**
anti,*anti*-**3**H^+–3	228.61	**-964.98**
anti,*anti*-**3**Na^+–AB	225.55	**-175.81**
anti,*anti*-**3**Na^+–BB'	225.46	**-178.69**
anti,*anti*-**3**Ag^+–BcB'c	222.68	**-268.55**
anti,*anti*-**3**Ag^+–AcBe	222.96	**-264.35**
anti,*anti*-**3**Ag^+–Af3'	215.30	**-251.12**
anti,*anti*-spiro(out)-**3**H^+	225.39	**-952.78**
anti,*syn*-spiro(out)-**3**H^+	214.96	**-952.49**
syn,*anti*-spiro(out)-**3**H^+	223.96	**-951.86**
syn,*syn*-spiro(out)-**3**H^+	193.81	**-983.44**

[a] Energies are relative to *anti*,*anti*-**3** plus the corresponding cation (H^+, Na^+, Ag^+) if necessary.

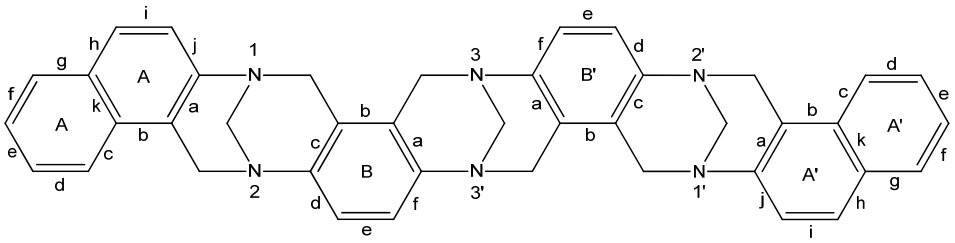
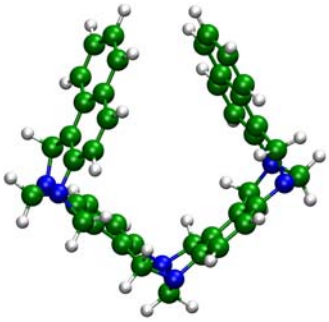
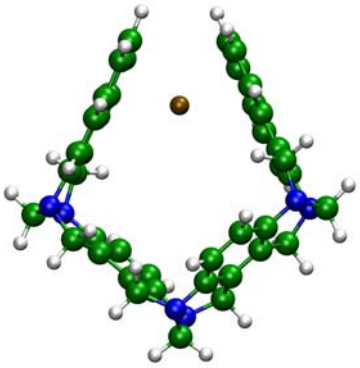


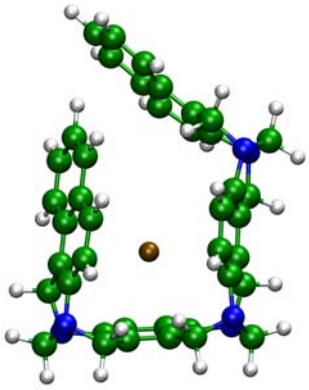
Figure S40. Notations used for distinguishing isomers of complexes of **3**. For *syn*,*anti*, the primed end of the molecule is in *anti* geometry.



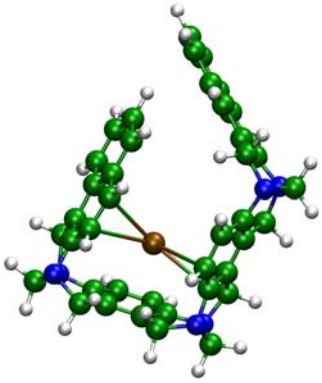
syn,*syn*-**3**



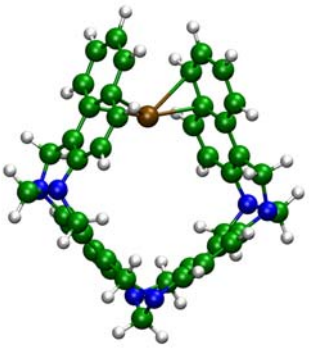
syn,*syn*-**3**Na^+–AA′



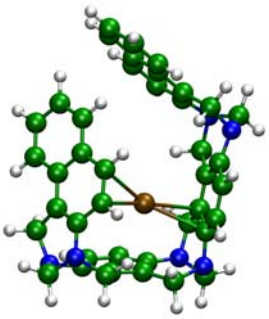
syn,*syn*-**3**Na^+–ABB′



syn,*syn*-**3**Ag^+–AiB′f

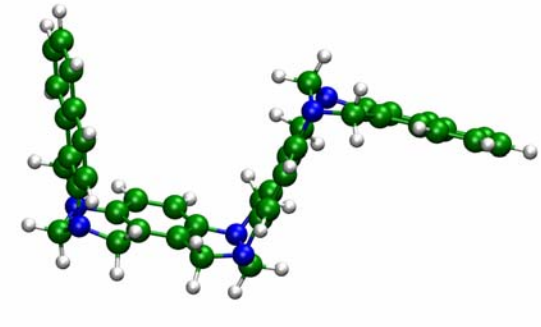


syn,*syn*-**3**Ag^+–AkA′g

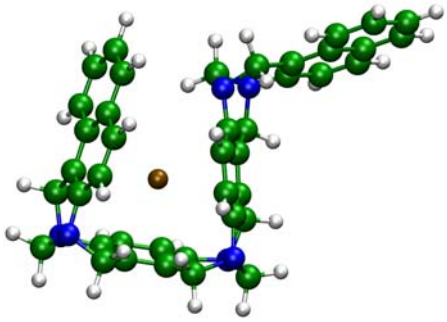


syn,*syn*-**3**Ag^+–AiB′a

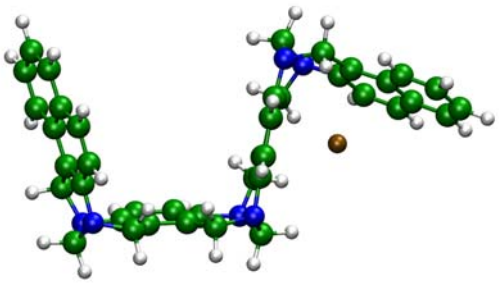
Figure S41. Various structures of complexes of **3**(continued on several next pages). Spiro structures are discussed in a separate section of the Supporting Information. Protonated TBs have geometries closely similar to the neutral molecule and are not shown here.



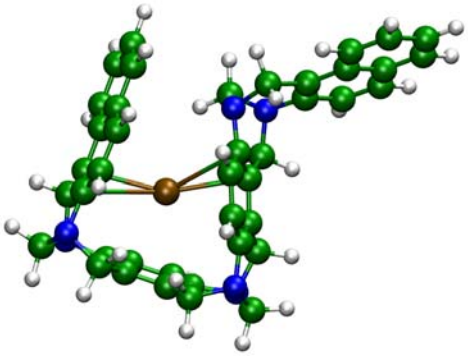
syn,anti-**3**



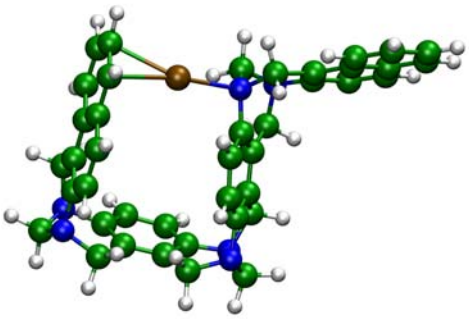
syn,anti-**3**Na^+–ABB′



syn,anti-**3**Na^+–A′B′



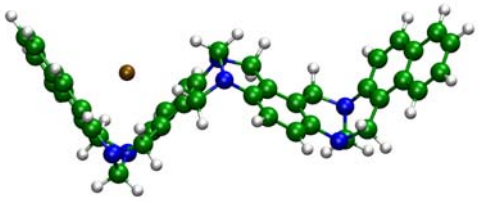
syn,anti-**3**Ag^+–AaB′c



syn,anti-**3**Ag^+–Af′

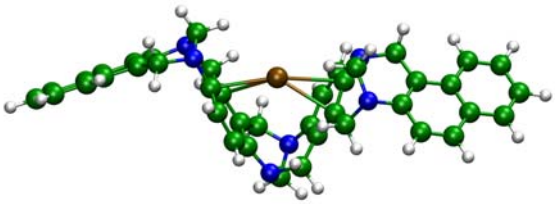
Figure S41. (continued from the previous page)

anti,anti-**3**

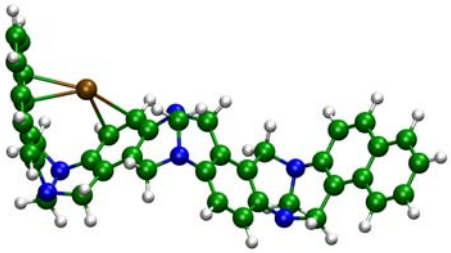


anti,anti-**3**Na^+–AB

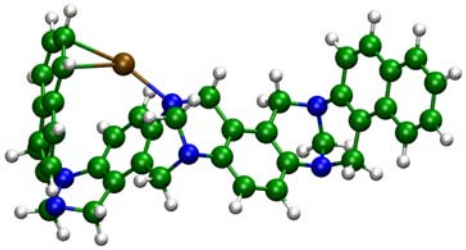
anti,anti-**3**Na^+–BB′



anti,anti-**3**Ag^+–BcB′c



anti,anti-**3**Ag^+–AcBe



anti,anti-**3**Ag^+–Af3′

Figure S41. (continued from the previous page)

Total energies for all calculated structures

Table S4. Electronic and zero-point vibrational energies of all structures relevant to bis-TB **2**. Data are given in atomic units.

	M06-2X/def2-SVP + SDD(f)		M06-2X/def2-TZVPP + SDD(2f,g)
Structure	Electronic energy	ZPVE	Electronic energy
syn-**2**	-1452.438985	0.516686	-1454.021746
syn-**2**H^+–in	-1452.818308	0.530660	-1454.401798
syn-**2**H^+–out	-1452.817177	0.530665	-1454.400696
syn-**2**Na^+	-1614.530465	0.518560	-1616.160351
syn-**2**Ag^+	-1599.163459	0.517975	-1600.739498
anti-**2**	-1452.439120	0.516778	-1454.021860
anti-**2**H^+–in	-1452.818351	0.530666	-1454.401822
anti-**2**H^+–out	-1452.817315	0.530656	-1454.400767
anti-**2**Na^+–π	-1614.514975	0.518280	-1616.147493
anti-**2**Na^+–N	-1614.509928	0.518420	-1616.141188
anti-**2**Ag^+	-1599.145759	0.518496	-1600.724048
anti-spiro(in)-**2**H^+	-1452.810779	0.529030	-1454.392761
syn-spiro(in)-**2**H^+	-1452.809705	0.529286	-1454.391871
anti-spiro(out)-**2**H^+	-1452.815294	0.529107	-1454.397446
syn-spiro(out)-**2**H^+	-1452.815505	0.529116	-1454.397714
Na^+	-162.006139	0.000000	-162.0567862
Ag^+	-146.593375	0.000000	-146.5933755
d1	-3198.318794	1.037029	-3201.468566
d2	-3198.317063	1.036215	-3201.464368
d3	-3198.273668	1.037580	-3201.425665
d4	-3198.308420	1.035814	-3201.457963
d5	-3198.299839	1.035615	-3201.451754
d6	-3198.288513	1.036318	-3201.440609
d7	-3198.300969	1.036553	-3201.448965
d8	-3198.298677	1.035751	-3201.449038

Table S5. Electronic and zero-point vibrational energies of all structures relevant to tris-TB **3**. Data are given in atomic units.

	M06-2X/def2-SVP + SDD(f)		M06-2X/def2-TZVPP + SDD(2f,g)
Structure	Electronic energy	ZPVE	Electronic energy
syn,*syn*-**3**	-1909.203011	0.676675	-1911.283068
syn,*syn*-**3**H^+–1	-1909.581914	0.690755	-1911.662537
syn,*syn*-**3**H^+–2	-1909.583854	0.690756	-1911.664545
syn,*syn*-**3**H^+–3	-1909.583889	0.690674	-1911.664713
syn,*syn*-**3**Na^+–AA'	-2071.294228	0.678338	-2073.424385
syn,*syn*-**3**Na^+–ABB'	-2071.296347	0.678492	-2073.423800
syn,*syn*-**3**Ag^+–AiB'f	-2055.928156	0.677841	-2058.002270
syn,*syn*-**3**Ag^+–AkA'g	-2055.920805	0.677465	-2057.995770
syn,*syn*-**3**Ag^+–AiB'a	-2055.928388	0.678117	-2058.002425
syn,*anti*-**3**	-1909.202636	0.676767	-1911.283050
syn,*anti*-**3**H^+–1	-1909.580240	0.690729	-1911.661337
syn,*anti*-**3**H^+–2	-1909.582492	0.690811	-1911.663659
syn,*anti*-**3**H^+–3	-1909.583378	0.690698	-1911.664599
syn,*anti*-**3**H^+–3'	-1909.583389	0.690617	-1911.664562
syn,*anti*-**3**H^+–2'	-1909.583179	0.690855	-1911.664425
syn,*anti*-**3**H^+–1'	-1909.580792	0.690756	-1911.661889
syn,*anti*-**3**Na^+–ABB'	-2071.299121	0.678903	-2073.426621
syn,*anti*-**3**Na^+–A'B'	-2071.278160	0.678275	-2073.408539
syn,*anti*-**3**Ag^+–AaB'c	-2055.932034	0.677845	-2058.004874
syn,*anti*-**3**Ag^+–Af2'	-2055.928902	0.678653	-2058.004483
anti,*anti*-**3**	-1909.203092	0.676825	-1911.283510
anti,*anti*-**3**H^+–1	-1909.580750	0.690760	-1911.661835
anti,*anti*-**3**H^+–2	-1909.582876	0.690711	-1911.664059
anti,*anti*-**3**H^+–3	-1909.583869	0.690855	-1911.665080
anti,*anti*-**3**Na^+–AB	-2071.278303	0.678267	-2073.408701
anti,*anti*-**3**Na^+–BB'	-2071.278759	0.678062	-2073.409593
anti,*anti*-**3**Ag^+–BcB'c	-2055.904055	0.677715	-2057.980061
anti,*anti*-**3**Ag^+–AcBe	-2055.901897	0.677882	-2057.978629
anti,*anti*-**3**Ag^+–Af3'	-2055.898292	0.678437	-2057.974143
anti,*anti*-spiro(out)-**3**H^+	-1909.578968	0.689142	-1911.658722
anti,*syn*-spiro(out)-**3**H^+	-1909.578933	0.689235	-1911.658704
syn,*anti*-spiro(out)-**3**H^+	-1909.578611	0.689146	-1911.658376
syn,*syn*-spiro(out)-**3**H^+	-1909.592117	0.690008	-1911.671266

Cartesian coordinates for all calculated structures

M06-2X/def2-SVP+SDD(f) fully optimized geometries, given in standard XYZ format: coordinates are Cartesian coordinates in the usual order, units are ångströms, first line indicates total number of atoms, second line is molecule name. Page numbers are omitted in this section to ease copying and pasting.

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 C -1.577657 0.745570 1.194974
 C -2.301409 1.866700 1.619794
 C -3.170206 0.423567 -0.614859
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 H 5.225144 0.260626 -2.347830
 H 6.248141 1.677744 -2.196992
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 H 0.821027 -1.317343 2.217632
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 H 1.259204 -1.480746 -2.125230
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 C -9.575115 0.026613 2.002559
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 C -6.419887 -1.868119 -1.464706
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 H -3.020780 -0.288075 -2.658196
 H -3.707454 -1.461822 -1.525459
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 H -4.234610 1.822918 -2.842884
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 H -9.476792 -3.184549 0.859164
 H -10.737873 -1.755761 2.444926
 H -10.135419 0.653735 2.697441
 H -8.302690 1.625635 1.392675
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anti-anti-3Ag+-Af3'
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 C -5.008434 1.421399 1.301162
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 C -4.986662 0.539262 2.418654
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 N -5.028041 -2.299937 -1.566191
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 C -3.080775 -1.006627 -2.183311
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 C -1.945455 -1.391843 0.343463
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 C -0.481387 0.576526 1.521555
 N -0.084301 -0.760175 1.826856
 C -1.235196 -1.641180 1.663838
 C 0.675556 0.719189 -0.560961
 C 1.503355 -0.438944 -0.034183
 C 1.095152 -1.141076 1.108412
 C 1.862535 -2.216660 1.571058
 C 2.697396 -0.786628 -0.687937
Ag -2.374583 2.320558 -0.127153
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 H -6.662016 -3.273226 -0.708701
 H -3.652821 -4.065216 0.871290
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 H 3.599787 -3.448048 1.233927
 H 1.543035 -2.745250 2.470620
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 H 7.039149 3.301452 -0.958803
 H 3.859751 -2.197746 -2.861626
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 H 8.792986 3.170475 0.761118
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 H 7.846318 -1.673466 1.426958
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 C -5.957342 1.604162 0.415176
 C -5.576875 2.469395 1.438246
 C -5.984238 3.806041 1.423663
 C -6.759414 4.303658 0.376188
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 C -6.982005 -0.133500 -1.645667
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 C -1.970853 -1.135602 -0.812989
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 N -0.098728 -0.236411 -2.151973
 C 0.070131 -1.624247 -2.535486
 N 0.008743 -2.485826 -1.363293
 C 0.863709 0.145776 -1.161626
 C 1.541551 -0.812972 -0.394251
 C 1.228571 -2.289435 -0.576273
 C 2.527069 -0.410100 0.522846
 C 1.145228 1.505218 -0.973723
 H 1.043667 -1.763201 -3.023243
 H -0.722487 -1.902857 -3.243987
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 H 4.797586 0.713144 3.345047
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 H 10.289426 1.530230 -2.190636
 H 8.892887 3.470171 -1.469319
 H 6.877843 3.123112 -0.117524
  82
anti,syn-spiro(out)-3H+
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 C -4.246887 3.794478 -1.909232
 C -5.366581 3.551142 -2.704775
 C -4.231215 0.757818 0.403432
 C -5.387203 -0.108732 0.852232
 C -6.454704 -0.407388 -0.063281
 C -6.634729 0.388025 -1.147383
 C -3.522756 1.343277 1.644443
 N -3.236196 0.266174 2.572914
 C -4.428727 -0.261192 3.131784
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 H -7.152729 -1.212246 0.172078
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 H -5.633464 4.241122 -3.505180
 H -7.021525 2.216471 -3.076350
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 H 0.555259 -1.532143 -3.617471
 H 5.049376 -0.427832 2.740491
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 H 6.674841 -0.662411 -1.221262
 H 4.163664 4.245847 3.152451
 H 3.893589 6.124713 1.557176
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  82
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 C -7.246694 0.789049 -1.222193
 C -8.071718 1.783088 -1.755252
 C -8.018626 3.089494 -1.269523
 C -5.389715 0.044120 0.333128
 C -4.891448 0.385568 1.720893
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C 1.603017 3.139732 -0.159959
C 1.438765 3.373579 1.239694
C 0.407352 4.242178 1.688633
C -0.448417 4.852139 0.797448
C -0.297571 4.616779 -0.590814
C 2.644545 2.273480 -0.621439
C 3.515192 1.707779 0.298308
C 3.332354 1.932377 1.694861
C 2.325954 2.734150 2.154383
C 2.793983 1.939328 -2.097586
N 3.701445 0.812990 -2.306398
C 4.898943 1.048173 -1.522400
N 4.604903 0.897761 -0.105316
C 3.103808 -0.445985 -1.989167
C 4.396472 -0.521323 0.178781
C 2.160719 -0.977843 -2.876911
H 3.168869 2.811892 -2.658947
H 1.814115 1.681967 -2.524212
H 5.368758 -1.038902 0.141115
H 4.025982 -0.618529 1.207936
H 1.982194 -0.458202 -3.819974
H 0.747379 -2.565376 -3.253480
H 4.046720 1.478583 2.383959
H 2.213928 2.925795 3.223649
H 5.680594 0.328597 -1.798536
H 5.266866 2.063431 -1.721961
H 0.312555 4.429024 2.761084
H -1.227120 5.527569 1.153616
H -0.964038 5.113197 -1.298027
H 0.816323 3.640029 -2.130968