Supporting information for

Vibrational CD study on the solution phase structures of the MacMillan catalyst and its corresponding iminium ion

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1. Comparison of 2·ClO_4 in $CDCl_3$ and methanol-d_4

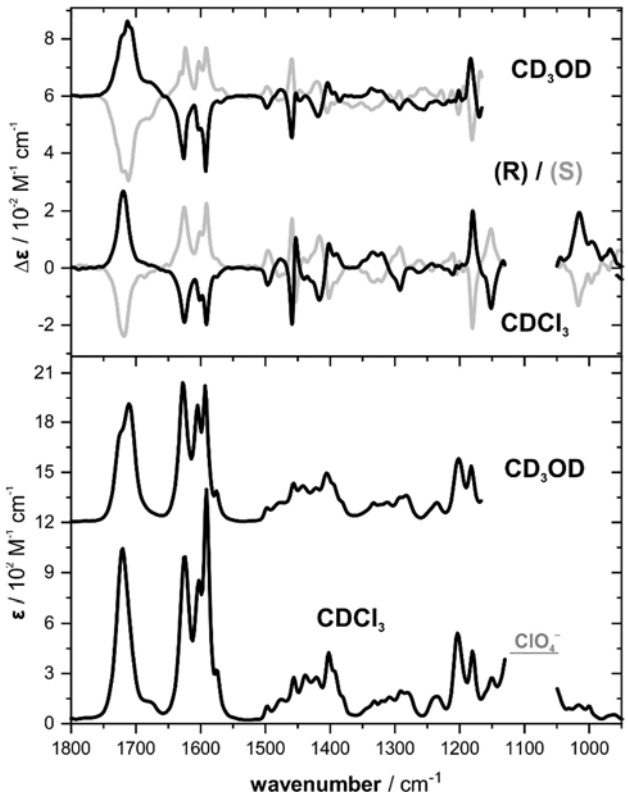


Figure S1. Comparison of the experimental IR and VCD spectra of **2**·ClO_4 in $CDCl_3$ (1800-1550 cm^{-1}: 0.07 M; 1550-950 cm^{-1}: 0.23 M) and methanol-d_4 (0.27 M) in a BaF_2 cell with 100 µm optical path length.

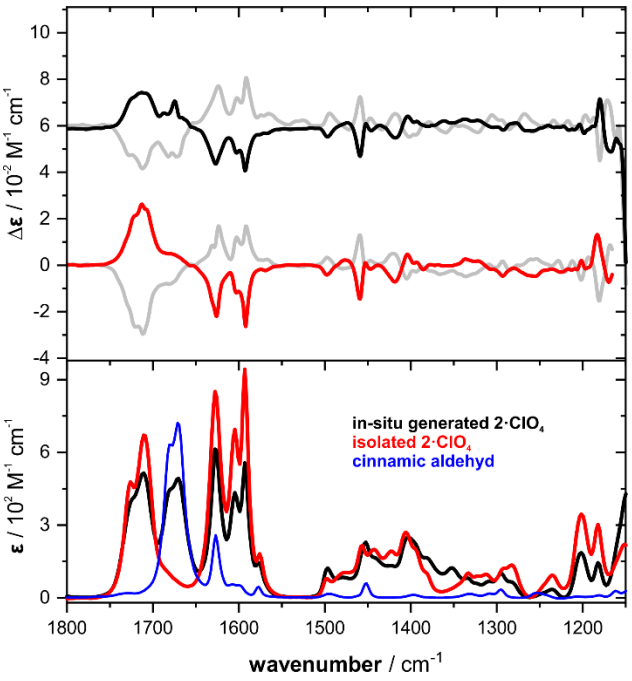


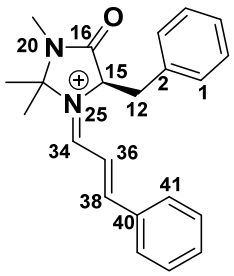
Figure S2. Comparison of the experimental IR and VCD spectra of **2**·ClO_4 in methanol-d_4 prepared *in-situ* from a 1:2 mixture of **1**·$HClO_4$ and cinnamic aldehyde with those obtained for the isolated salt. To show that residual aldehyde can also be observed in the IR, the IR spectrum of pure cinnamic aldehyde is shown as well.

2. Conformational analysis of 2

Table S1. Conformational analysis of iminium ion **2** at B3LYP/6-31+G(2d,p)/IEFPCM(**$CHCl_3$**) level of theory. Angle definitions α-ϕ are reported in Scheme S1. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ε	ϕ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
2b	4.5	-52.1	-81.7	-1.4	179.8	-0.2	0.0[a)]	0.0[a)]	60.8	44.7
2a	12.8	72.1	-102.1	2.1	-177.2	-179.9	0.65	0.38	20.3	23.5
2c	10.5	177.4	112.2	-1.6	179.9	0.5	1.20	0.56	8.1	17.4
2d	7.4	139.4	55.4	0.0	-178.2	-1.9	1.41	1.18	5.6	6.0
2e	8.4	67.1	71.5	176.6	178.1	-0.2	1.68	1.30	3.5	5.0
2f	1.7	-54.3	-80.0	-179.5	178.7	-0.4	2.13	1.55	1.7	3.3
2g	7.4	170.7	-68.6	178.1	179.1	-1.0	4.03	3.62	0.1	0.1
2h	3.2	-51.5	-79.1	-6.5	175.4	152.6	5.66	6.71	0.0	0.0
2i	11.2	68.2	-100.8	-5.5	177.2	-29.8	5.95	6.31	0.0	0.0
2j	6.1	-50.9	-82.1	4.5	-176.8	-150.7	6.50	6.76	0.0	0.0
2k	9.5	174.5	108.1	-6.6	175.9	152.9	6.55	5.91	0.0	0.0
2l	13.3	70.0	-100.0	6.7	-176.2	31.9	6.59	6.58	0.0	0.0
2m	6.3	140.4	-122.1	-4.1	178.1	-30.3	6.99	6.94	0.0	0.0
2n	3.7	-53.1	-80.8	-6.6	-14.8	-1.5	7.00	6.58	0.0	0.0
2o	9.3	69.2	72.7	172.2	172.5	-29.1	7.02	7.34	0.0	0.0
2p	11.7	172.0	113.6	4.0	-176.6	-151.3	7.47	7.58	0.0	0.0
2q	8.4	136.3	-123.3	4.2	-176.4	29.3	7.74	7.87	0.0	0.0
2r	2.3	-56.1	-80.1	175.6	174.4	-29.0	8.07	8.55	0.0	0.0
2s	9.7	146.0	43.2	-2.0	0.1	-0.6	8.63	8.75	0.0	0.0
2t	11.4	175.9	97.7	-6.7	-13.5	172.5	9.02	8.55	0.0	0.0
2u	11.3	70.7	73.8	178.3	172.7	-154.1	9.06	8.96	0.0	0.0
2v	4.7	-57.0	-79.3	-176.5	177.8	29.6	9.17	9.61	0.0	0.0
2w	8.9	168.6	-74.8	173.1	173.7	-30.1	9.32	9.44	0.0	0.0
2x	13.3	66.5	86.7	-7.3	-12.8	174.5	9.48	9.06	0.0	0.0
2y	-9.5	88.0	47.2	-167.1	-171.3	28.1	10.22	10.71	0.0	0.0
2z	6.5	172.2	-73.8	-176.7	-177.1	-150.4	10.25	10.22	0.0	0.0
2za	7.6	67.6	75.6	176.3	-22.7	-6.2	11.25	10.82	0.0	0.0
2zb	2.5	-55.6	-81.1	-179.5	-9.4	-4.0	12.50	12.45	0.0	0.0
2zc	3.3	-52.9	-79.1	-1.7	-39.3	-27.5	13.22	13.80	0.0	0.0
2zd	9.1	166.7	-73.1	176.9	-17.6	177.1	13.82	13.61	0.0	0.0
2ze	12.7	69.0	82.3	-3.9	-42.9	-27.4	15.10	15.72	0.0	0.0
2zf	6.9	144.5	54.3	-3.3	-41.6	-24.5	15.44	15.63	0.0	0.0
2zg	9.9	174.7	-74.0	-177.2	-80.5	-26.5	21.09	20.88	0.0	0.0
2zh	7.3	-64.8	111.3	-168.0	-76.3	-26.1	22.18	22.95	0.0	0.0

a) referenced to E(**2b**) = -1037.63449 hartree and G(**2b**) = -1037.6884 hartree.



α = (20,16,15,25) δ = (15,25,34,36)

β = (25,15,12,2) ε = (25,34,36,38)

γ = (15,12,2,1) ϕ = (36,38,40,41)

Scheme S1. Torsional angle definitions of **2**.

Table S2. Conformational analysis of iminium ion **2** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-ϕ are reported in Scheme S1. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ε	ϕ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
2b	4.8	-52.9	-81.7	-1.2	179.6	0.2	0.0[a)]	0.0[a)]	48.8	43.5
2a	12.7	71.6	-101.7	0.9	-177.3	179.1	0.49	0.28	21.4	27.2
2c	10.8	178.5	112.7	-1.7	179.6	0.7	0.51	0.64	20.5	14.8
2d	7.3	139.7	54.5	-0.3	-179.4	-0.8	1.30	0.91	5.5	9.4
2e	8.3	67.9	72.5	176.2	178.2	0.5	1.85	1.95	2.1	1.6
2f	2.2	-54.8	-80.3	-179.8	179.0	-0.2	2.10	1.57	1.4	3.1
2g	7.1	170.8	-68.7	178.2	179.7	0.5	3.01	2.76	0.3	0.4
2h	3.8	-53.3	-80.4	-6.0	175.6	152.3	5.39	5.83	0.0	0.0

a) referenced to E(**2b**) = -1037.649638 hartree and G(**2b**) = -1037.704123 hartree.

3. Additional data for 1

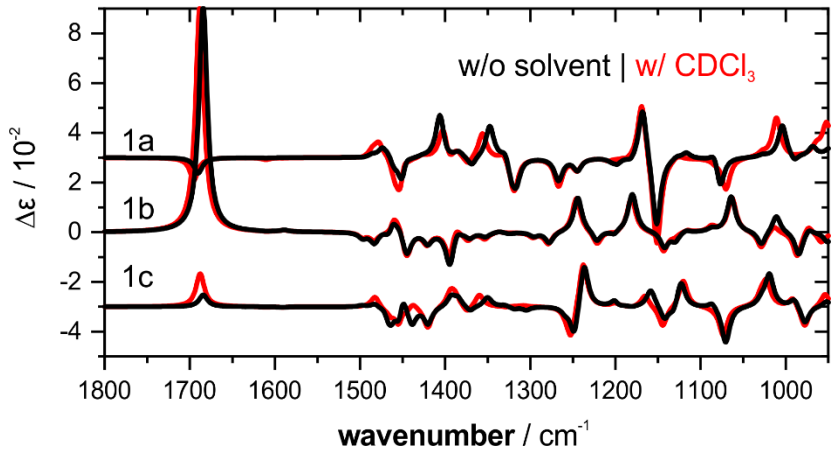


Figure S3. Comparison of single-conformer spectra of **1** and **1**·$CDCl_3$

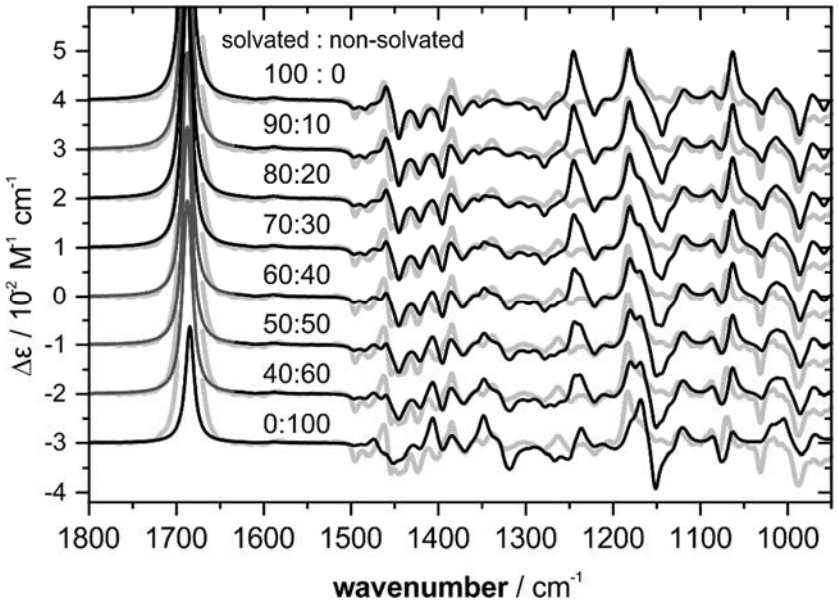


Figure S4. Mixture spectra of **1**·$CDCl_3$ and monomeric **1**, which show that the solvated species is dominating.

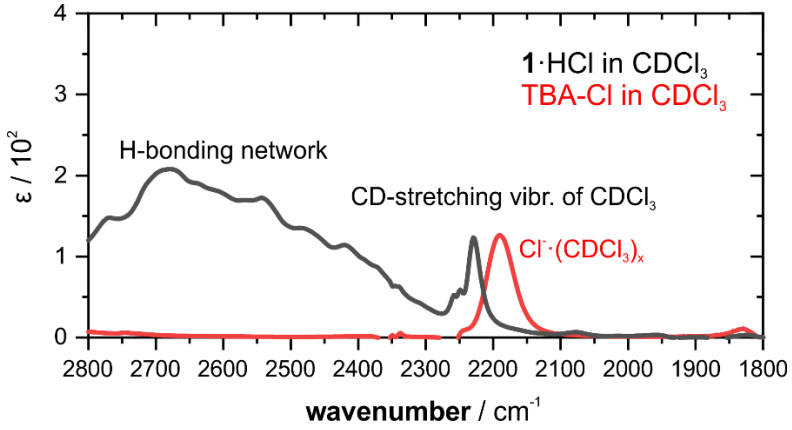


Figure S5. Comparison of the IR spectrum of **1**·HCl with that of tetrabutyl ammonium chloride (TBA-Cl) in the range of the C-D stretching vibrations. In TBA-Cl, the chloride is assumed to be fully solvated, hence the shift of the CD-vibration should be characteristic for a $CDCl_3$-solvated Cl^-. As the CD-band is less strongly shifted for **1**·HCl, we assumed that the chloride is not fully solvated and instead H-bonded to the cation.

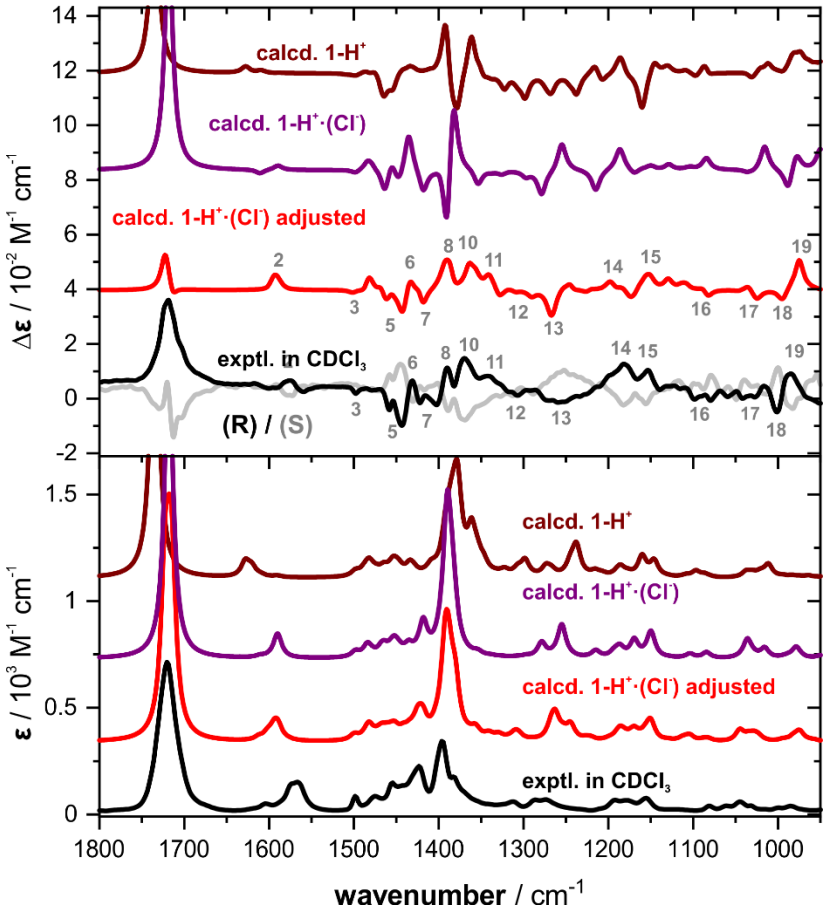


Figure S6. Comparison of the IR and spectrum of **1**·HCl recorded in $CDCl_3$ with the computed spectra of the bare cation **1**-H^+, of **1**-$H^+(Cl^-)$ and the manually adjusted conformational distribution of **1**-$H^+(Cl^-)$.

4. Conformational analysis of 1 and 1-H$^+$

Table S3. Conformational analysis of neutral catalyst **1** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

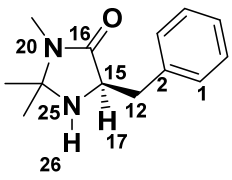
Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a	-13.6	32.9	68.2	80.0	0.00	0.00	29.7	30.9
1b	-10.8	152.3	-53.6	98.0	0.41	0.78	14.9	8.3
1c	-11.2	151.6	67.1	73.8	0.01	0.21	29.4	21.8
1d	4.7	-7.8	69.2	79.9	0.50	0.17	12.7	23.1
1e	-11.2	151.6	77.3	158.6	1.13	0.83	4.4	7.6
1f	-11.5	30.9	-54.8	96.4	1.31	1.30	3.2	3.4
1g	-10.5	150.7	164.5	115.0	1.42	1.57	2.7	2.2
1h	-13.3	32.6	167.3	115.3	1.69	1.70	1.7	1.7
1i	8.4	-12.9	170.3	111.5	1.95	2.06	1.1	1.0

a) referenced to E(**1a**) = -690.76044 hartree and G(**1a**) = -690.80427 hartree

Table S4. Conformational analysis of neutral catalyst **1** at B3LYP/6-31+G(2d,p)/IEFPCM(**$CHCl_3$**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a	-13.5	33.1	69.1	82.4	0.0[a)]	0.0[a)]	32.9	34.5
1b	-10.8	152.3	-53.3	98.3	0.18	0.54	24.4	13.8
1c	-10.8	150.9	68.0	74.4	0.27	0.37	21.0	18.4
1d	3.3	-4.9	70.6	83.5	0.63	0.28	11.4	21.4
1e	-11.5	151.9	78.1	153.4	1.16	1.01	4.7	6.3
1f	-8.8	26.2	-57.5	90.4	1.43	1.52	2.9	2.6
1g	-10.6	150.6	162.8	110.8	1.84	1.84	1.5	1.5
1h	-12.8	32.0	165.2	108.1	2.17	2.05	0.8	1.1
1i	8.3	-12.8	169.9	109.5	2.53	2.70	0.5	0.4

a) referenced to E(**1a**) = -690.753245 hartree and G(**1a**) = -690.796946 hartree



α = (20,16,15,25) γ = (25,15,12,2)

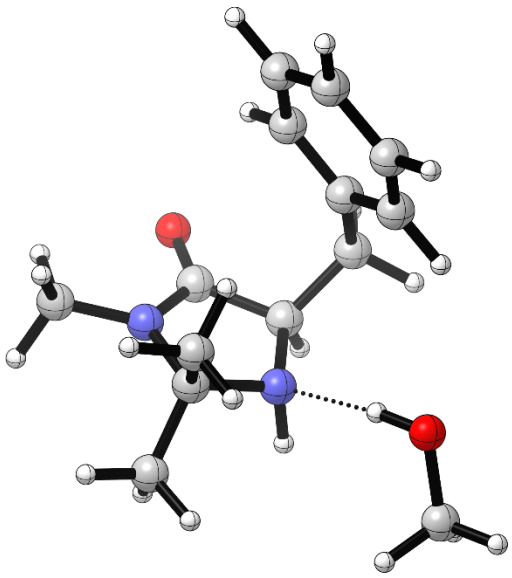
β = (26,25,15,17) δ = (15,12,2,1)

Scheme S2. Torsional angle definitions of **1**.

Table S5. Conformational analysis of neutral catalyst **1 explicitly solvated with CD_3OD** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	H-bond direction	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a	NH -> OH	-12.3	31.8	69.2	78.7	2.71	1.12	0.4	6.4
1a	OH -> N	-16.5	35.9	72.8	78.6	0.98	1.91	7.8	1.7
1b	NH -> OH	-11.2	153.2	-54.2	98.6	3.58	2.63	0.1	0.5
1b	OH -> N	-10.6	152.6	-53.7	98.4	0.00	0.50	40.8	18.0
1c	NH -> OH	-12.8	154.0	70.4	78.0	3.06	2.69	0.2	0.4
1c	OH -> N	-9.9	150.3	67.7	72.4	0.06	0.43	36.8	20.4
1e	NH -> OH	-11.5	151.8	77.0	159.9	1.18	0.00	5.5	42.2
1f	NH -> OH	-10.7	30.6	-56.1	94.3	3.78	2.76	0.1	0.4
1g	NH -> OH	-11.0	150.7	163.8	115.5	4.31	2.97	0.0	0.3
1g	OH -> N	-10.3	151.2	165.4	116.4	1.05	1.06	7.0	7.1
1h	NH -> OH	-12.9	33.3	166.8	116.2	4.14	2.94	0.0	0.3
1h	OH -> N	-14.4	32.6	165.4	114.8	2.25	1.90	0.9	1.7
1i	NH -> OH	8.6	-12.4	169.9	113.3	4.28	2.59	0.0	0.5
1j	OH -> N	3.7	-5.9	-61.6	101.1	2.83	3.80	0.3	0.1

a) referenced to E(**1b**) = -806. 472778 hartree and G(**1e**) = -806. 525949 hartree

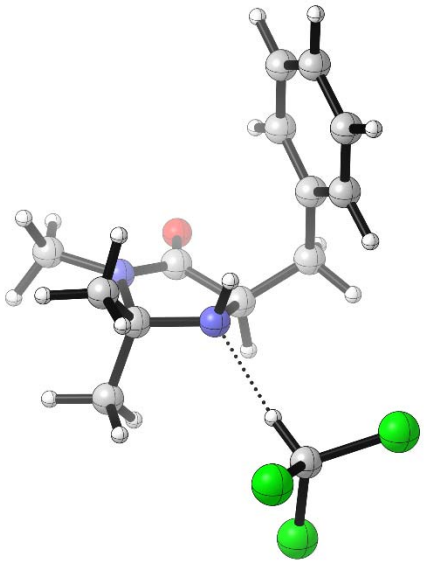


Structure of 1b(NH -> OH)

Table S6. Conformational analysis of neutral catalyst **1 explicitly solvated with $CDCl_3$** at B3LYP/6-31+G(2d,p)/IEFPCM(**$CHCl_3$**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a · $CDCl_3$	-18.4	39.4	77.1	76.5	1.87	1.79	3.2	3.0
1b · $CDCl_3$	-10.7	152.3	-53.1	98.9	0.0[a)]	0.0[a)]	74.7	62.9
1c · $CDCl_3$	-8.5	148.9	69.0	71.3	0.94	1.14	15.3	9.1
1d · $CDCl_3$	5.6	-11.1	75.2	71.5	2.20	1.77	1.8	3.2
1g · $CDCl_3$	-10.4	151.2	162.7	109.9	1.76	0.69	3.8	19.5
1h · $CDCl_3$	-14.6	32.5	163.4	109.5	2.93	2.56	0.5	0.8
1i · $CDCl_3$	9.2	-16.4	166.6	107.9	2.78	2.28	0.7	1.3

a) referenced to E(**1a**) = -2110.032498 hartree and G(**1a**) = -2110.0901 hartree



Structure of 1b · $CDCl_3$

Table S7. Conformational analysis of cationic catalyst **1-H$^+$** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$	-11.7	31.4	63.9	67.0	0.13	0.00	40.8	57.5
1b-H$^+$	-10.7	30.2	-51.0	97.1	0.00	0.27	51.2	36.3
1d-H$^+$	7.2	-9.0	58.8	73.5	1.38	1.90	5.0	2.3
1g-H$^+$	-12.4	33.0	166.7	113.5	1.80	1.79	2.5	2.8
1i-H$^+$	8.5	-10.4	171.3	110.8	2.60	2.42	0.6	1.0

a) referenced to E(**1b-H$^+$**) = -691.190674 hartree and G(**1b-H$^+$**) = -691.234205 hartree

Table S8. Conformational analysis of cationic catalyst **1-H$^+$** at B3LYP/6-31+G(2d,p)/IEFPCM(**CHCl$_3$**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

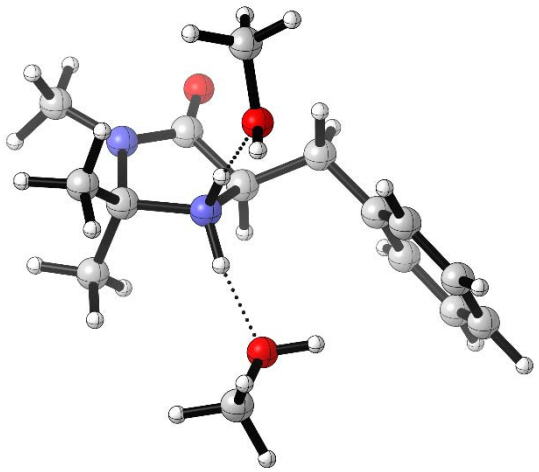
Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$	-11.6	32.1	61.7	73.8	0.68	0.46	23.2	30.2
1b-H$^+$	-10.8	30.8	-49.2	95.6	0.00	0.00	72.6	65.9
1d-H$^+$	7.2	-9.7	57.5	74.0	1.72	1.81	4.0	3.1
1g-H$^+$	-12.8	34.2	161.3	102.8	3.53	3.40	0.2	0.2
1i-H$^+$	8.0	-11.1	168.7	106.4	3.89	2.76	0.1	0.6

a) referenced to E(**1b-H$^+$**) = -691.164202 hartree and G(**1b-H$^+$**) = -691.206743 hartree

Table S9. Conformational analysis of cationic catalyst **1-H$^+$ explicitly solvated with two CD$_3$OD** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	H-bond direction	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$·(CD$_3$OD)$_2$	2x (NH -> OH)	-14.9	37.7	72.6	77.8	0.0[a)]	0.0[a)]	91.7	56.8
1g-H$^+$·(CD$_3$OD)$_2$	2x (NH -> OH)	-13.3	34.6	164.6	115.0	1.82	0.20	4.2	40.6
1b-H$^+$·(CD$_3$OD)$_2$	2x (NH -> OH)	-4.8	21.5	-59.5	98.9	1.84	1.83	4.1	2.6

a) referenced to E(**1a-H$^+$**) = -922.621527 hartree and G(**1a-H$^+$**) = -922.680971 hartree



Structure of 1a-H$^+$·(CD$_3$OD)$_2$

Table S10. Conformational analysis of cationic catalyst **1-H$^+$ explicitly solvated with one chloride and one CD_3OD** at B3LYP/6-31+G(2d,p)/IEFPCM(**methanol**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$·(Cl$^-$)$^{@proS}$(CD_3OD)	-12.279	33.658	76.696	66.052	0.10	1.45	18.8	5.3
1a-H$^+$·(Cl$^-$)$^{@proR}$(CD_3OD)	-14.283	37.249	83.085	71.236	0.37	1.81	11.8	2.9
1b-H$^+$·(Cl$^-$)$^{@proS}$(CD_3OD)	-10.587	32.895	-51.15	98.52	0.11	0.0 [a)]	18.3	61.5
1d-H$^+$·(Cl$^-$)$^{@proR}$(CD_3OD)	8.842	-11.366	68.808	64.218	1.46	2.97	1.9	0.4
1g-H$^+$·(Cl$^-$)$^{@proS}$(CD_3OD)	-11.069	32.427	167.081	115.223	0.0[a)]	0.69	22.1	19.1
1g-H$^+$·(Cl$^-$)$^{@proR}$(CD_3OD)	-9.949	30.892	166.286	114.861	0.72	1.94	6.6	2.3
1i-H$^+$·(Cl$^-$)$^{@proR}$(CD_3OD)	9.696	-10.281	170.743	112.228	0.84	1.76	5.3	3.1
1x-H$^+$·(Cl$^-$)$^{@proS}$(CD_3OD)	2.247	4.843	-58.997	101.537	0.55	2.06	8.8	1.9
1x-H$^+$·(Cl$^-$)$^{@proR}$(CD_3OD)	3.871	1.577	-61.315	100.899	1.30	2.31	2.5	1.2
1y-H$^+$·(Cl$^-$)$^{@proS}$(CD_3OD)	-1.496	12.026	75.857	64.904	1.00	1.95	4.1	2.3

a) referenced to E(**1g-H$^+$**) = - 1267.303039 hartree and G(**1b-H$^+$**) = - 1267.36034 hartree

Table S11. Conformational analysis of cationic catalyst **1-H$^+$ explicitly including one chloride** at B3LYP/6-31+G(2d,p)/IEFPCM(**$CHCl_3$**) level of theory. Angle definitions α-δ are reported in Scheme S2. Relative zero-point corrected and Gibbs free energies, ΔE_{ZPC} and ΔG_{298K}, are reported in kcal/mol and the corresponding Boltzmann populations in percentage.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$(Cl$^-$)$^{@proR}$	-16.0	37.7	74.7	79.8	2.82	3.17	0.8	0.4
1a-H$^+$(Cl$^-$)$^{@proS}$	-7.2	28.3	67.0	69.4	2.59	2.60	1.2	1.1
1b-H$^+$(Cl$^-$)$^{@proS}$	-11.0	33.9	-50.2	97.8	0.0[a)]	0.0[a)]	94.9	93.3
1d-H$^+$(Cl$^-$)$^{@proR}$	5.8	-13.7	98.7	80.9	5.16	5.07	0.0	0.0
1d-H$^+$(Cl$^-$)$^{@proS}$	7.7	-8.7	58.4	73.3	2.45	2.89	1.5	0.7
1g-H$^+$(Cl$^-$)$^{@proR}$	-13.5	33.4	164.1	106.3	4.80	4.82	0.0	0.0
1g-H$^+$(Cl$^-$)$^{@proS}$	-11.9	35.1	163.4	107.8	2.45	1.83	1.5	4.3
1i-H$^+$(Cl$^-$)$^{@proR}$	11.0	-18.8	166.7	106.3	4.47	4.33	0.0	0.1
1z-H$^+$(Cl$^-$)$^{@proR}$	7.0	-9.2	-67.4	103.9	4.94	5.14	0.0	0.0

a) referenced to E(**1b-H$^+$**) = -1151.575932 hartree and G(**1b-H$^+$**) = -1151.623232 hartree

Table S12. Adjusted conformational distribution of cationic catalyst **1-H$^+$ explicitly including one chloride**, obtained by removing conformer **1b** from the distribution. See discussion in the main text for details.

Conf.	α	β	γ	δ	ΔE_{ZPC}	ΔG_{298K}	p(ΔE)	p(ΔG)
1a-H$^+$(Cl$^-$)$^{@proR}$	-16.0	37.7	74.7	79.8	0.37	1.34	15.7	6.6
1a-H$^+$(Cl$^-$)$^{@proS}$	-7.2	28.3	67.0	69.4	0.14	0.78	23.3	17.2
1b-H$^+$(Cl$^-$)$^{@proS}$								
1d-H$^+$(Cl$^-$)$^{@proR}$	5.8	-13.7	98.7	80.9	2.71	3.24	0.3	0.3
1d-H$^+$(Cl$^-$)$^{@proS}$	7.7	-8.7	58.4	73.3	0.00	1.06	29.3	10.6
1g-H$^+$(Cl$^-$)$^{@proR}$	-13.5	33.4	164.1	106.3	2.35	2.99	0.6	0.4
1g-H$^+$(Cl$^-$)$^{@proS}$	-11.9	35.1	163.4	107.8	0.0[a)]	0.0[a)]	29.4	63.8
1i-H$^+$(Cl$^-$)$^{@proR}$	11.0	-18.8	166.7	106.3	2.02	2.51	1.0	0.9
1z-H$^+$(Cl$^-$)$^{@proR}$	7.0	-9.2	-67.4	103.9	2.49	3.31	0.4	0.2

a) referenced to E(**1g-H$^+$**) = -1151.572028 hartree and G(**1g-H$^+$**) = -1151.62032 hartree