Supporting information for

Anion-binding of a chiral tris(2-aminoethyl)amine-based tripodal thiourea: A spectroscopic and computational study

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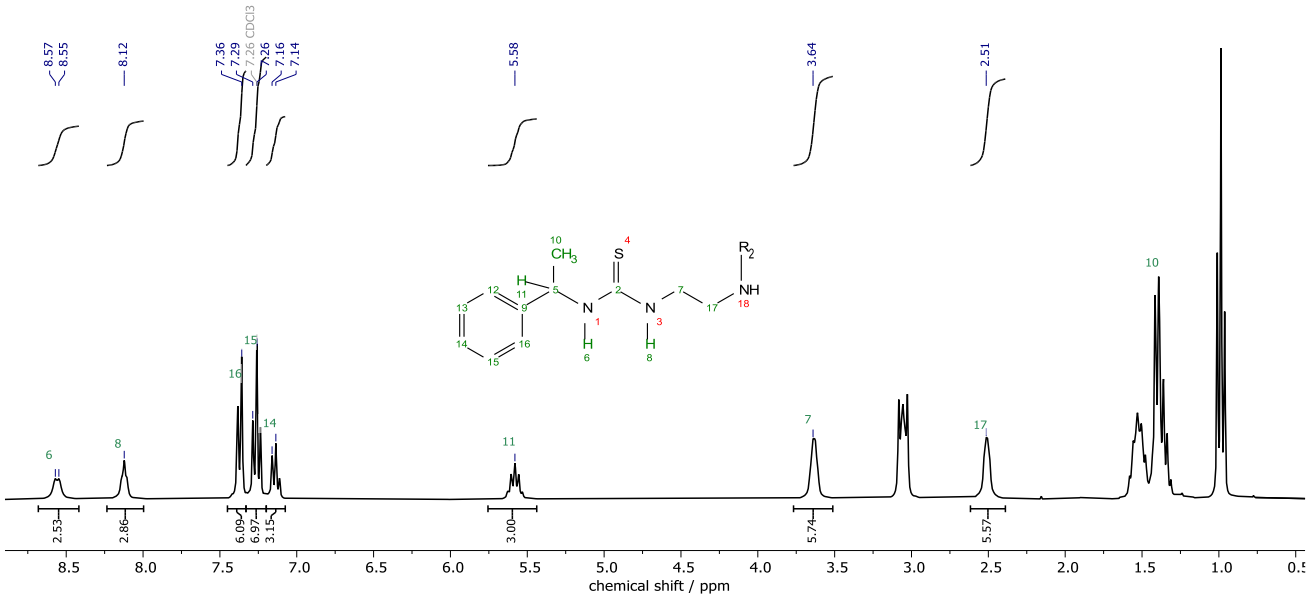
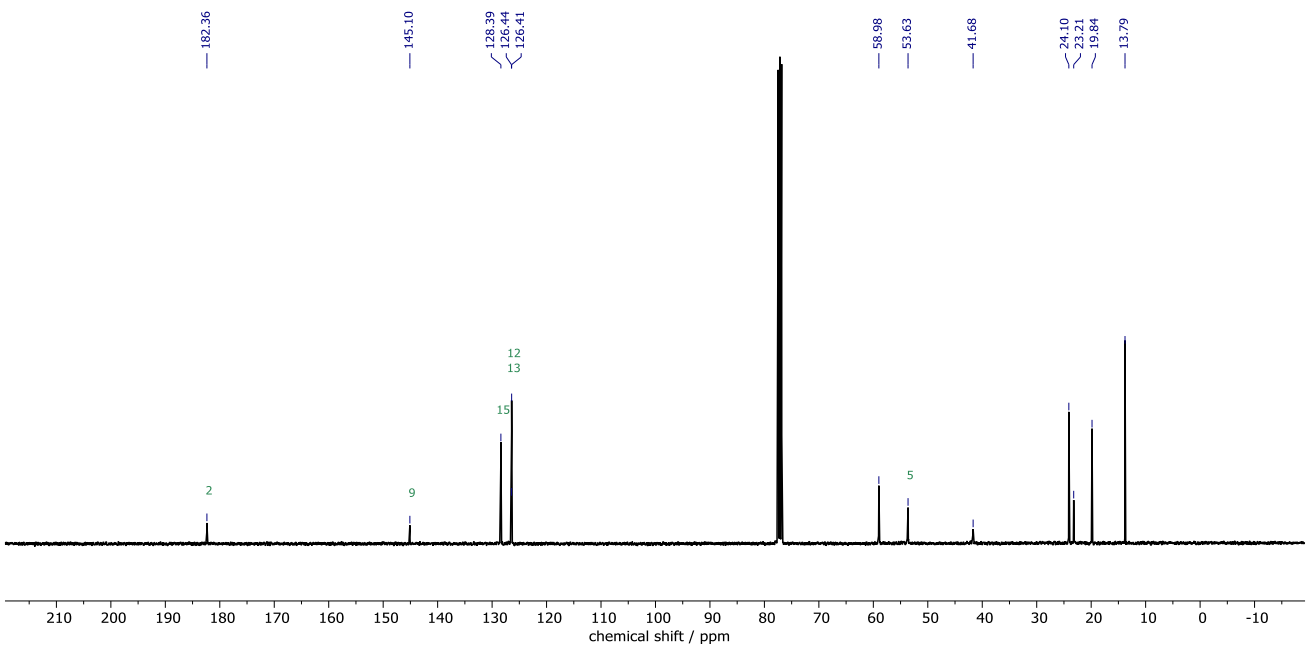
1. NMR spectra

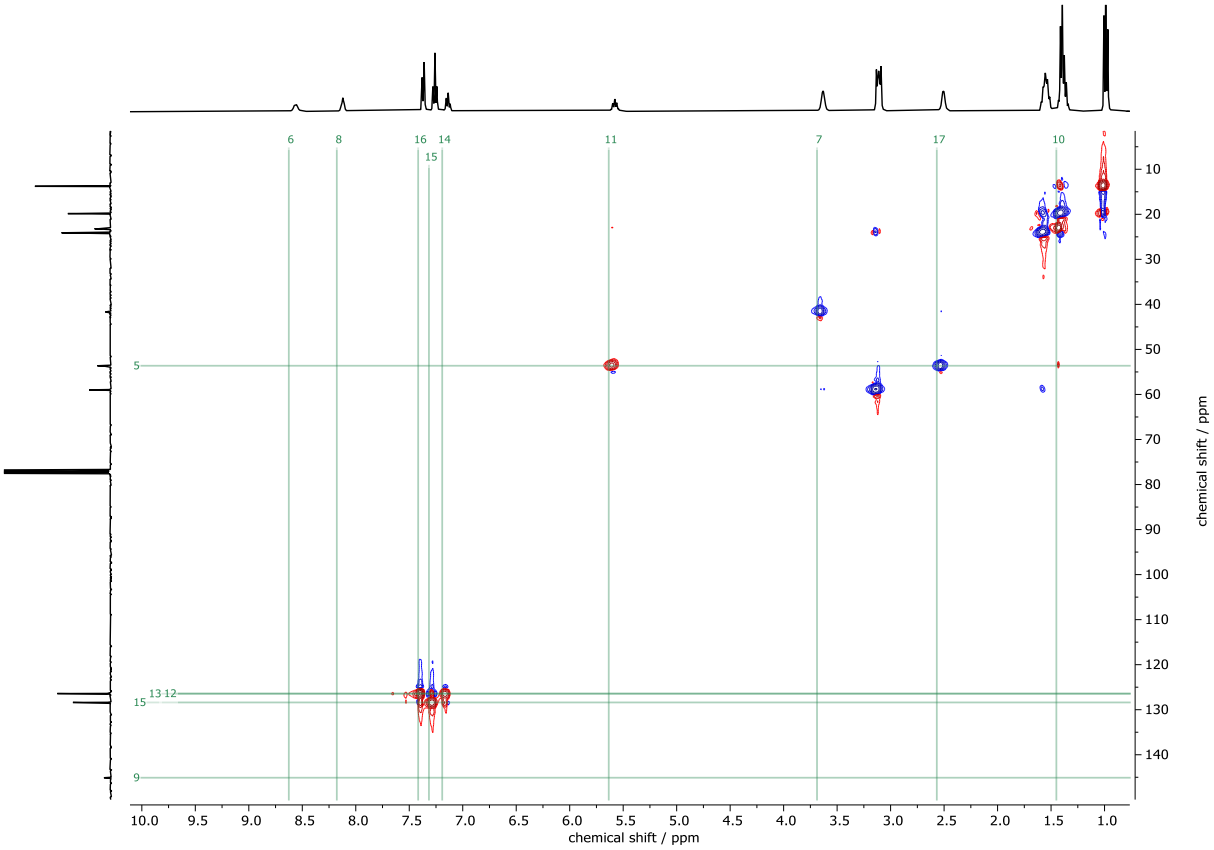
^{1}H-NMR of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



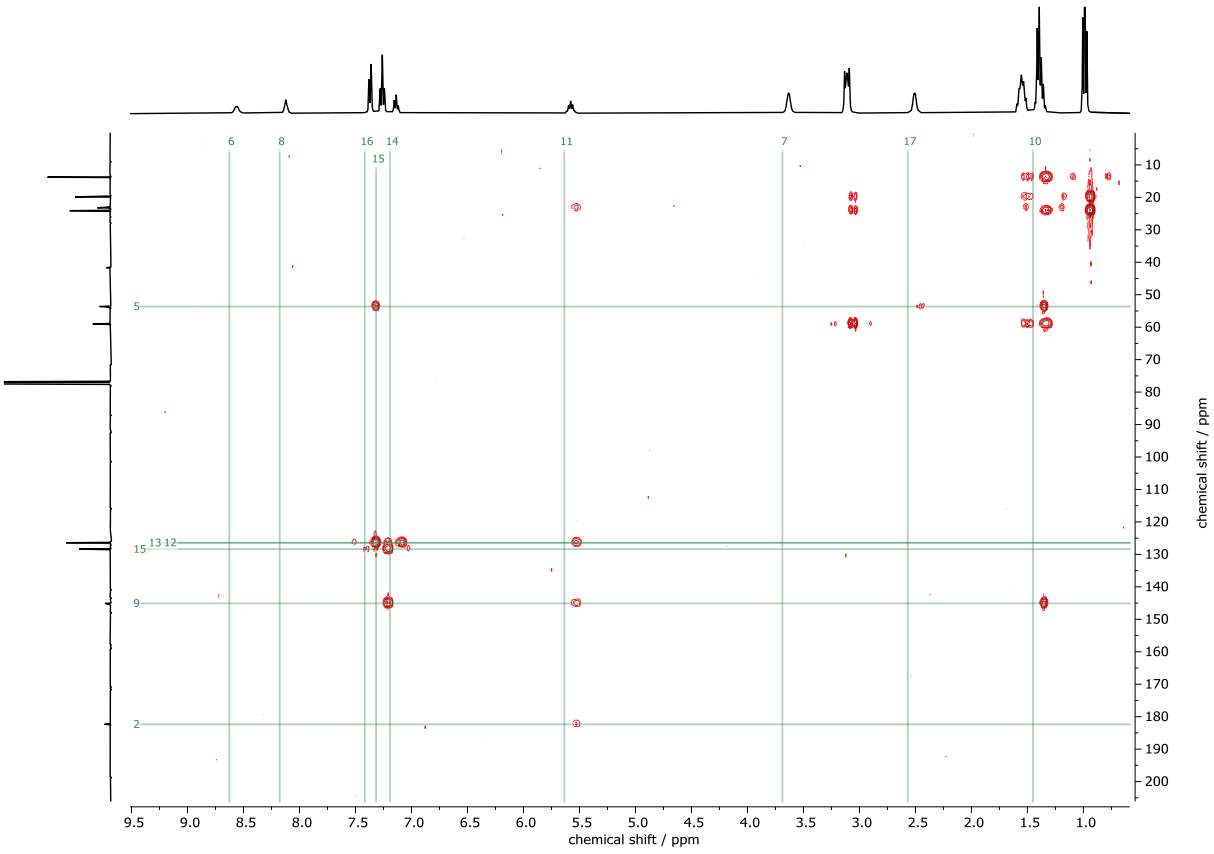
^{13}C-NMR of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



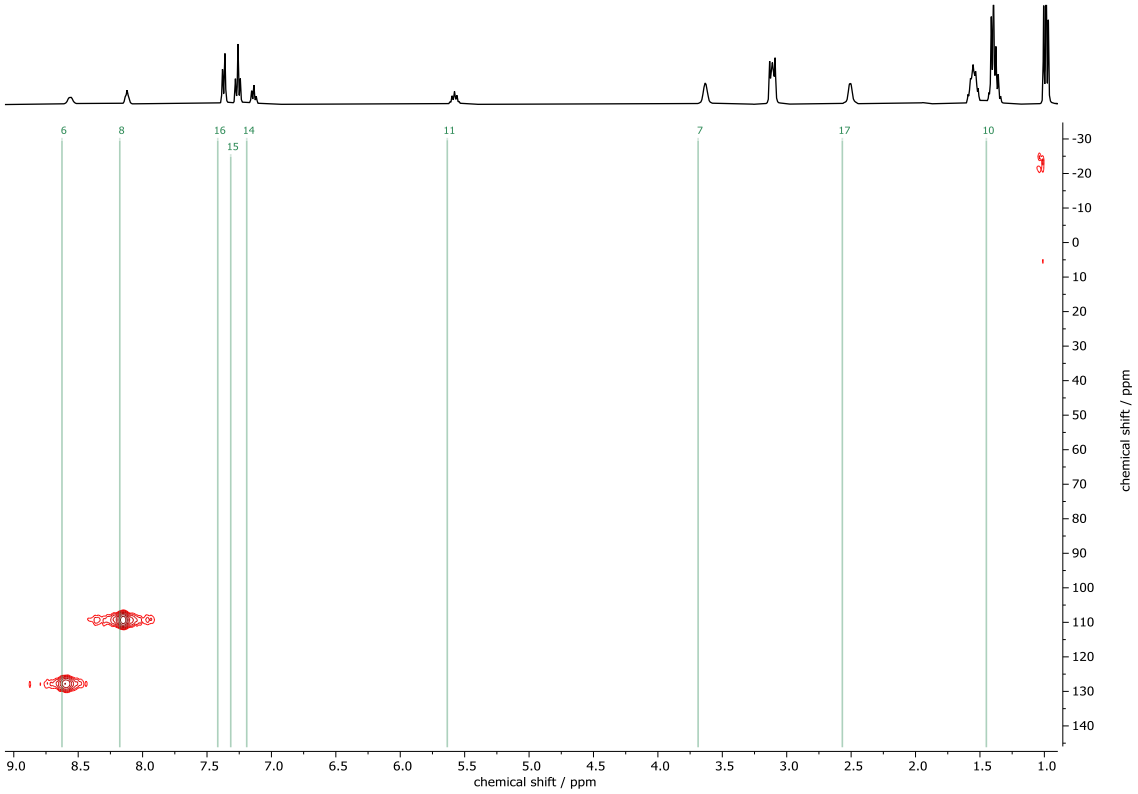
{^{1}H,^{13}C}-HSQC of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



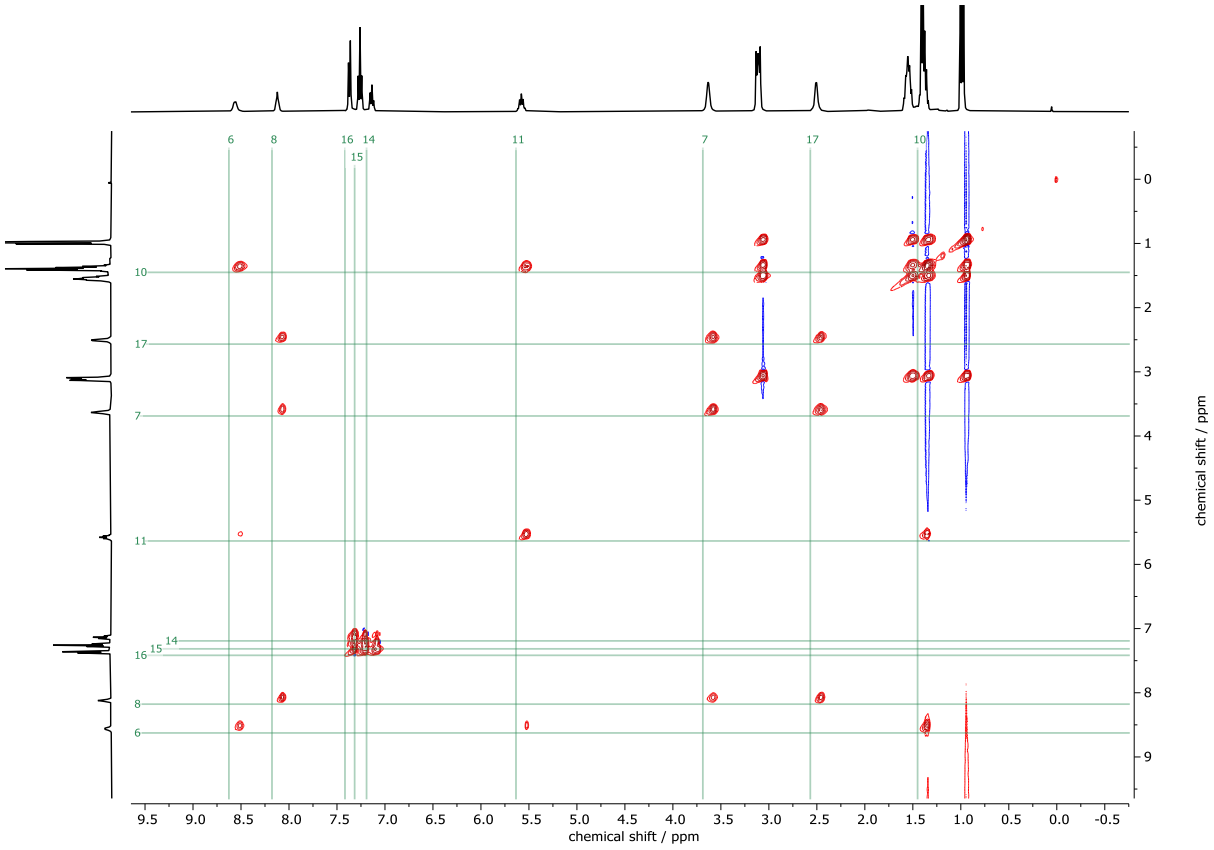
{^{1}H,^{13}C}-HMBC of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



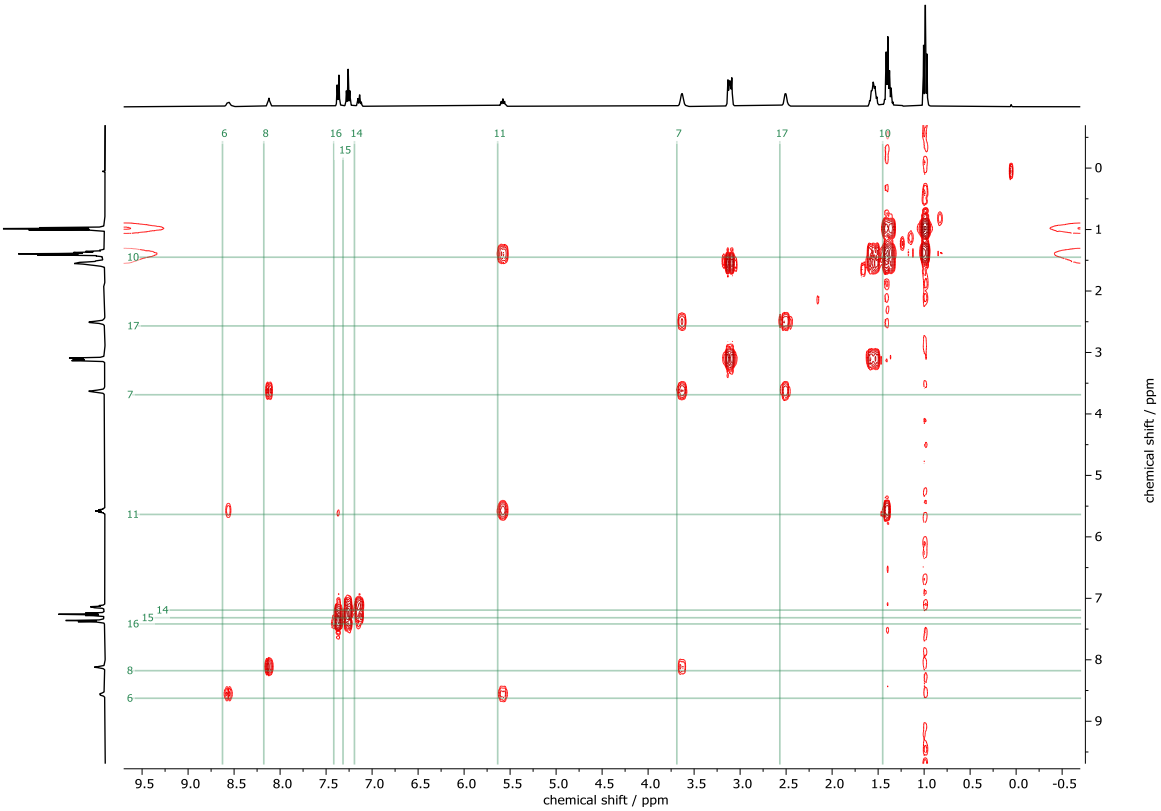
{^{1}H,^{15}N}-HSQC of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



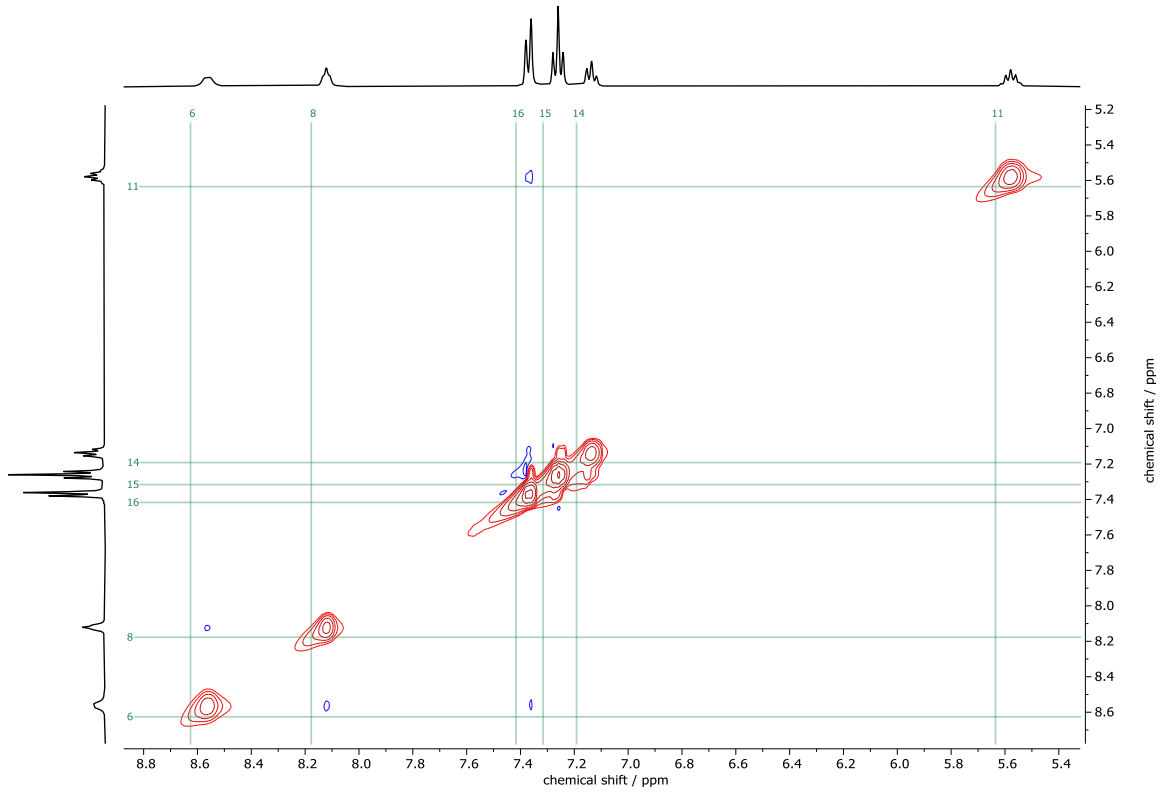
TOCSY of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



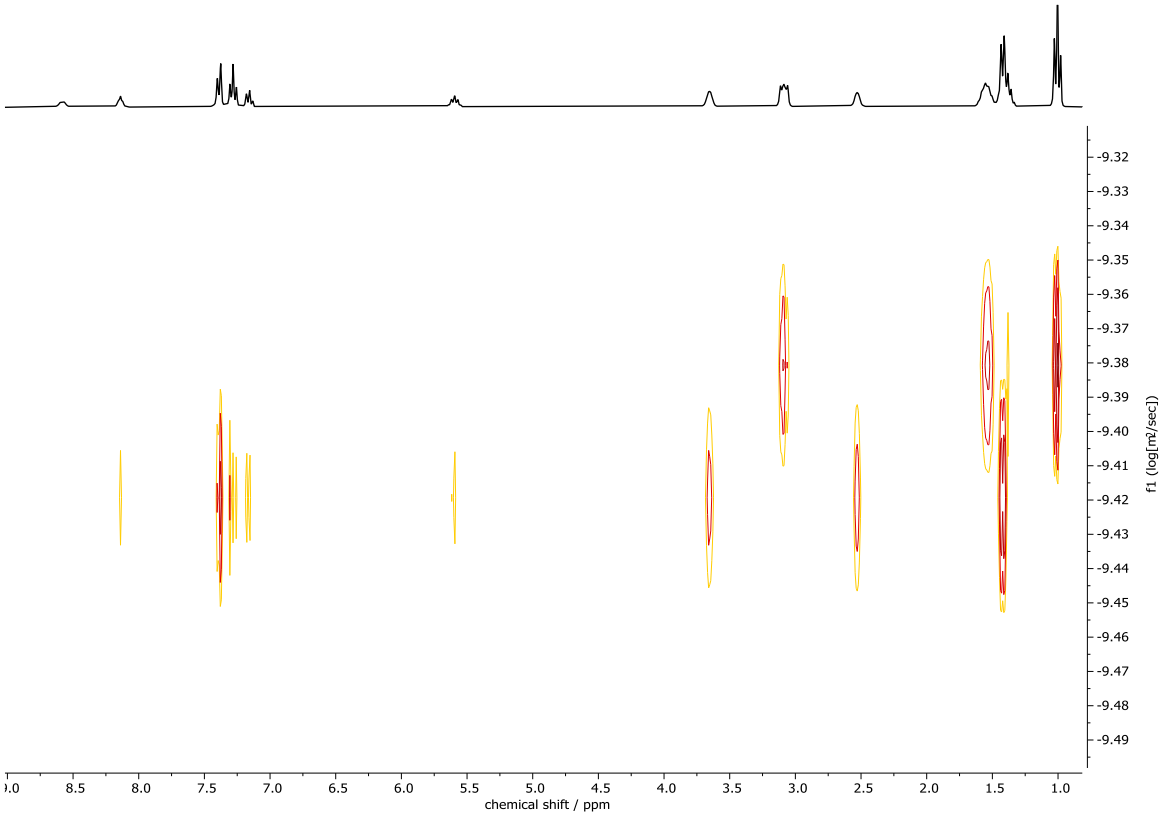
COSY of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



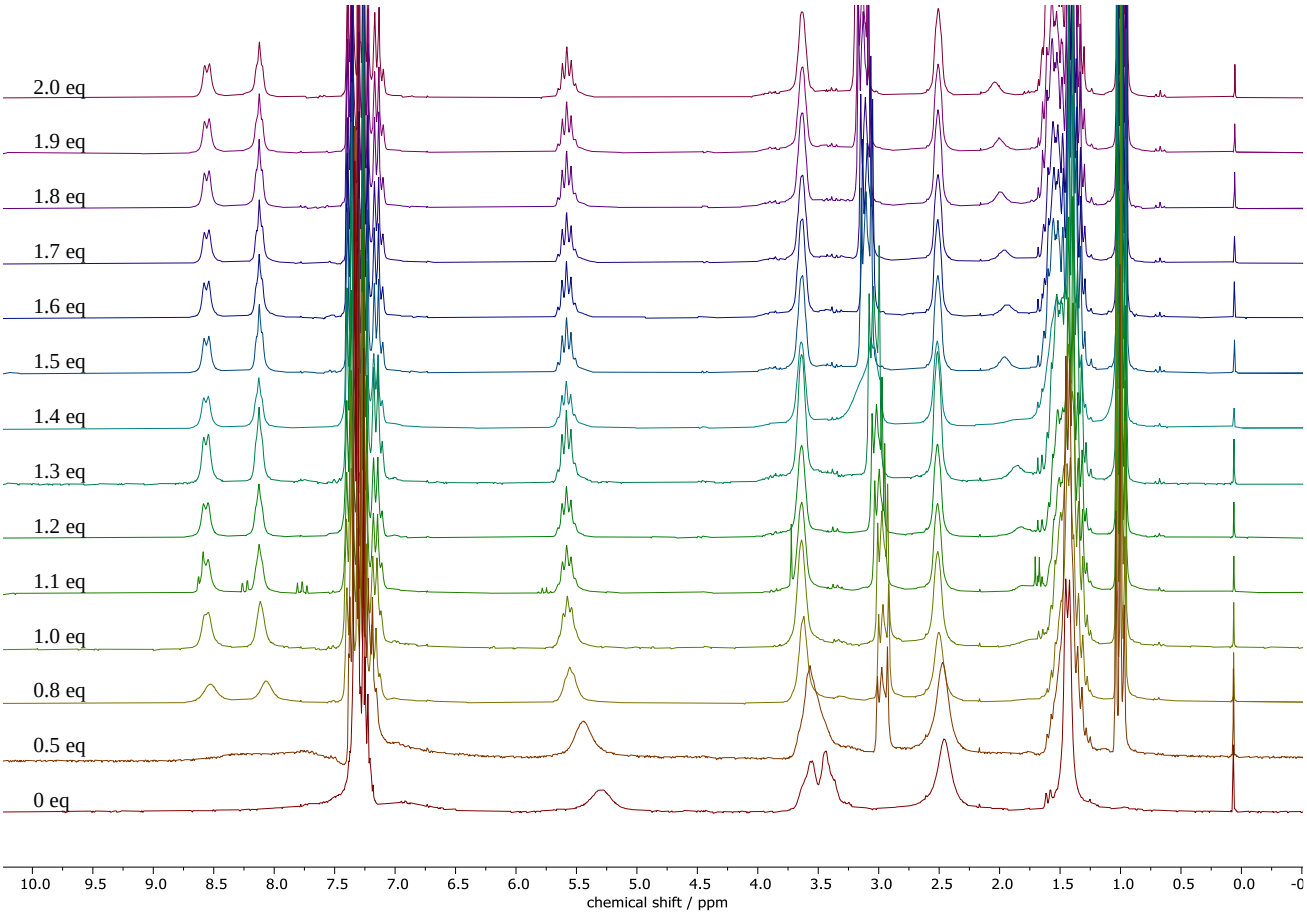
NOESY of 1+TBA-Cl (1:1.5) in $CDCl_3$ (400 MHz, 31 mM)



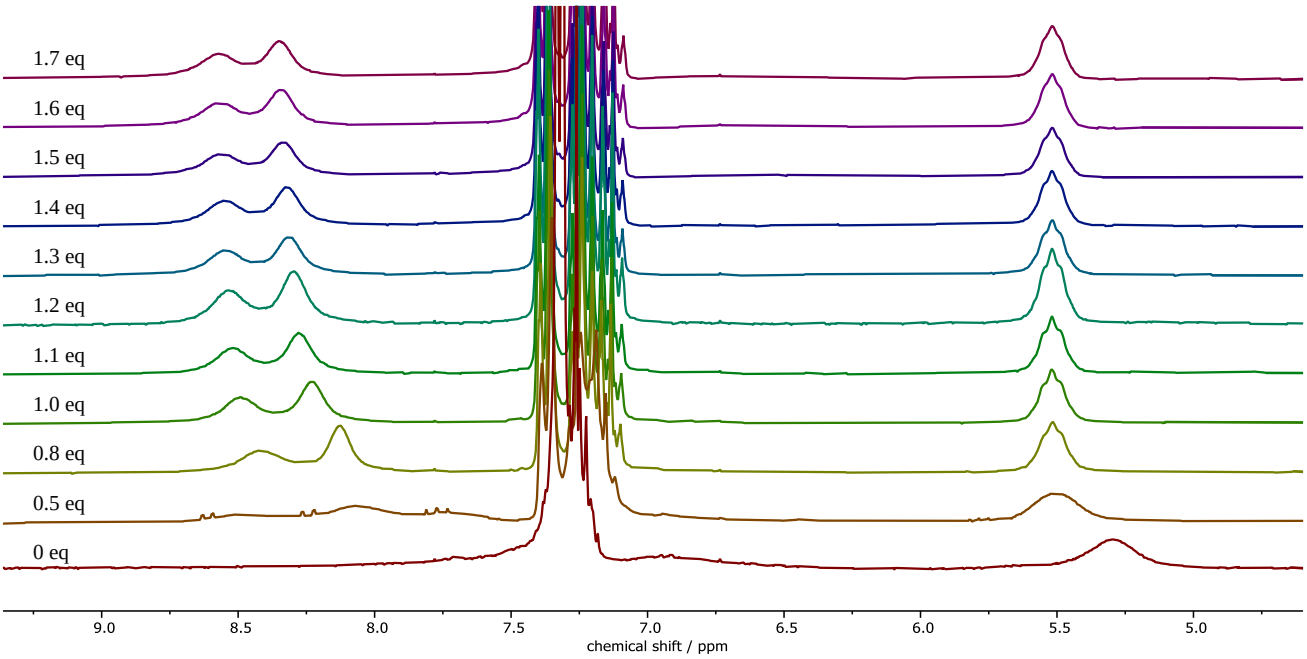
DOSY-NMR of 1+TBA-Cl (1:1.5) (400 MHz, 31 mM)



Titration of 1 with TBA-Cl (200 MHz, 78 mM)

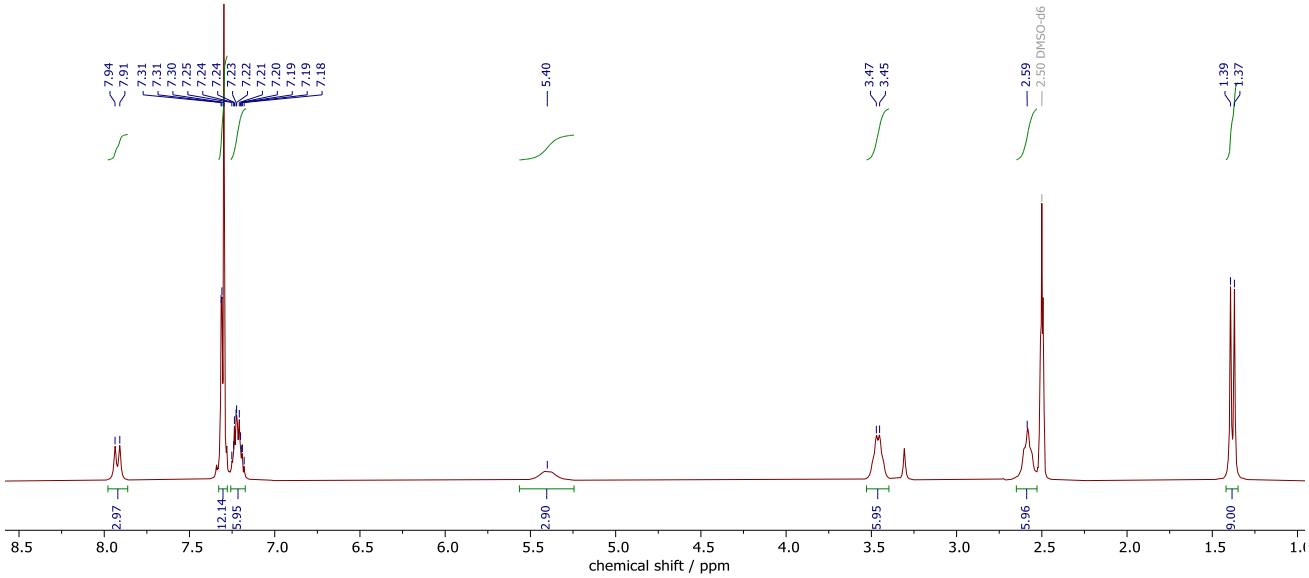


Titration of 1 with TBA-HSO_4 (200 MHz, 78 mM)

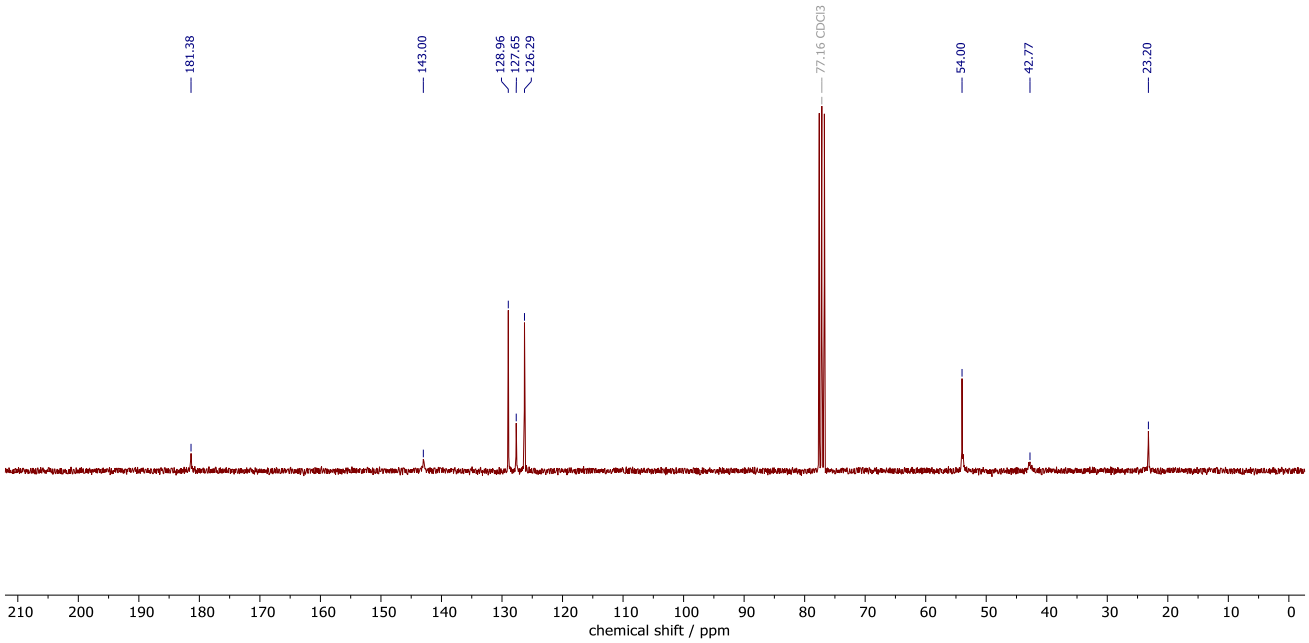


3. Analytical data for structure confirmation

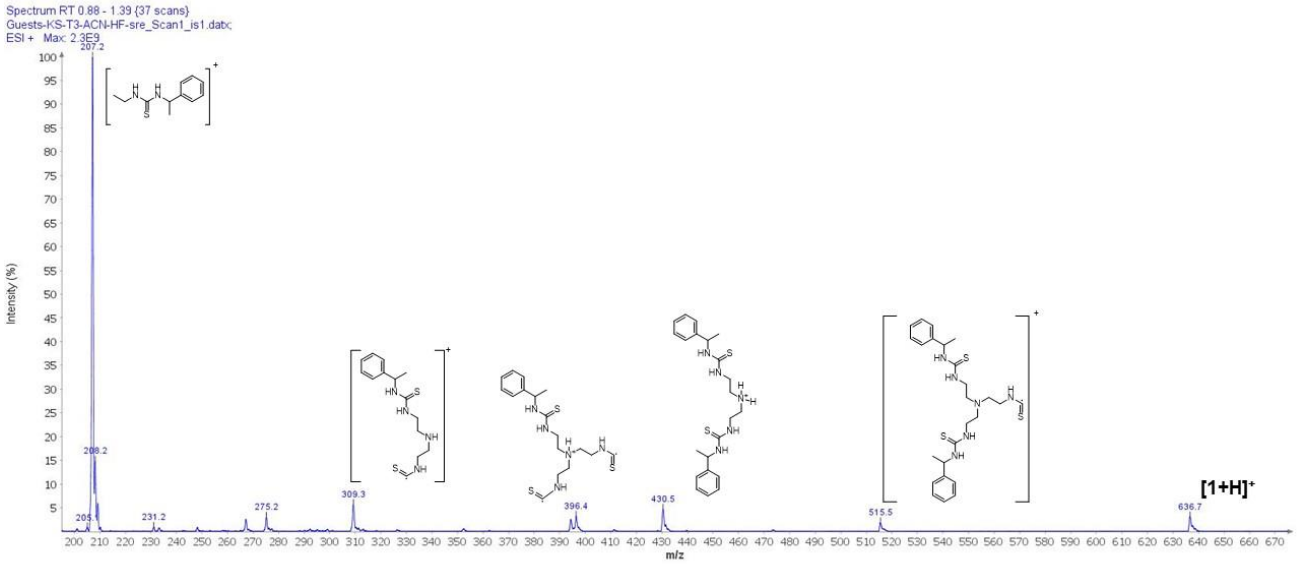
^{1}H-NMR of 1 in DMSO-d6 (200 MHz, 78 mM)



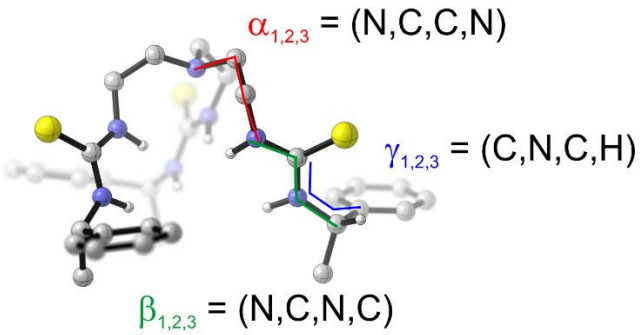
^{13}C-NMR of 1 in $CDCl_3$ (300 MHz, 78 mM)



ESI-MS of 1 in Acetonitrile/MeOH



3. Computed conformer energies and conformational distributions



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

Table S1. Key torsional angles of the optimized geometries of **1**·Cl^-. Angle definitions shown in Scheme S1.

	TREN head group				Thiourea moieties				α-methylbenzyl arms		
Conformer	**α1**	**α2**	**α3**		**β1**	**β2**	**β3**		**γ1**	**γ2**	**γ3**
CL_AAAAAA_P_c1	**63.9**	**64.9**	**64.4**	**P**	**176.3**	**176.0**	**177.4**	AA AA AA	**33.2**	**32.1**	**32.1**
CL_AAAAAA_M_c1	**-64.8**	**-65.0**	**-65.2**	**M**	**176.5**	**176.7**	**176.3**	AA AA AA	**31.4**	**31.5**	**30.0**
CL_AAAAAA_P_c2	63.5	64.7	65.4	**P**	176.7	177.0	-175.3	AA AA AA	32.5	30.9	-20.2
CL_AAAAAA_M_c2	-65.5	-64.9	-65.8	**M**	176.3	176.8	-177.6	AA AA AA	32.4	33.0	-15.3
CL_AAAAAA_P_c3	64.7	65.3	65.3	**P**	178.7	-175.5	-174.6	AA AA AA	31.9	-15.9	-19.2
CL_AAAAAA_M_c3	-65.4	-65.5	-64.4	**M**	-177.6	176.1	-178.3	AA AA AA	-13.6	32.1	-7.2
CL_AAAAAA_PPM_c1	-56.6	61.9	65.7	**M/PP**	177.5	178.8	176.1	AA AA AA	29.3	35.6	31.8
CL_AAAAAA_MMP_c1	56.7	-66.8	-60.8	**P/MM**	175.9	176.0	177.9	AA AA AA	29.4	31.3	31.8
CL_AAAAAA_P_c4	65.0	65.8	65.8	**P**	-174.3	-173.6	-174.2	AA AA AA	-13.4	-17.6	-18.3
CL_AAAAAA_M_c5	-65.0	-46.6	-62.9	**M**	179.4	178.8	-179.9	AA AA AA	178.2	178.6	177.9
CL_AAAAAA_P_c5	62.9	62.7	65.0	**P**	178.7	178.9	179.3	AA AA AA	178.9	178.8	178.5
CL_AAAAAA_MMP_c2	56.1	-66.1	-61.4	**P/MM**	177.2	177.5	-179.2	AA AA AA	179.4	178.7	177.8
CL_AAAAAS_M_c1	-66.4	-62.2	-81.1	**M**	174.7	175.5	8.5	AA AA AS	30.4	27.4	-39.4
CL_AAAAAS_P_c1	59.1	65.8	82.6	**P**	174.8	174.8	6.1	AA AA AS	32.1	28.5	-27.9
CL_AAAAAS_P_c2	60.5	66.7	82.0	P	-176.5	-175.2	4.1	AA AA AS	-16.9	-21.3	-26.2
CL_AAASAS_P_c1	62.2	83.3	76.0	**P**	174.2	-19.5	-18.5	AA AS AS	29.5	50.0	49.9
CL_AAASAS_P_c2	61.1	81.8	77.3	P	-176.6	-22.7	-18.3	AA AS AS	-17.6	52.9	50.2
CL_AAASAS_M_c1	-63.3	-78.4	-83.2	**M**	175.2	10.8	16.5	AA AS AS	23.9	-41.1	-46.1
CL_ASASAS_P_c2	78.8	79.1	78.6	**P**	-19.6	-20.3	-19.5	AS AS AS	50.1	50.8	50.3
CL_ASASAS_M_c1	-79.1	-78.8	-79.8	**M**	16.6	18.1	17.6	AS AS AS	-44.5	-46.2	-46.7

Table S2. Relative conformer energies (in kcal/mol) of **1**·Cl^- obtained considering all conformers together and sorted by individual conformer families.

	All conformers				Individual families			
Conformer	**ΔE_{ZPC}**	**ΔG_{298K}**	**$\chi(\Delta E)$**	**$\chi(\Delta G)$**	**ΔE_{ZPC}**	**ΔG_{298K}**	**$\chi(\Delta E)$**	**$\chi(\Delta G)$**
Cl_AAAAAA_P_c1	**0.0**[a)]	0.35	43.6	31.2				
Cl_AAAAAA_M_c1	0.12	**0.0** [a)]	35.5	55.9				
Cl_AAAAAA_P_c2	0.90	2.65	9.5	0.6				
Cl_AAAAAA_M_c2	1.15	1.25	6.3	6.8				
Cl_AAAAAA_P_c3	1.92	1.93	1.7	2.1				
Cl_AAAAAA_M_c3	2.04	2.11	1.4	1.6				
Cl_AAAAAA_PPL_c1	2.31	3.31	0.9	0.2				
Cl_AAAAAA_MMR_c1	2.36	2.57	0.8	0.7				
Cl_AAAAAA_P_c4	2.89	2.59	0.3	0.7				
Cl_AAAAAA_M_c5	15.70	17.87	0.0	0.0				
Cl_AAAAAA_P_c5	16.00	17.91	0.0	0.0				
Cl_AAAAAA_MMR_c2	17.76	20.17	0.0	0.0				
Cl_AAAAAS_M_c1	4.11	4.27	0.0	0.0	0.00	0.00	54.6	48.7
Cl_AAAAAS_P_c1	4.28	4.28	0.0	0.0	0.16	0.01	41.4	47.6
Cl_AAAAAS_P_c2	5.97	5.86	0.0	0.0	1.85	1.59	2.4	3.3
Cl_AAASAS_P_c1	6.33	7.27	0.0	0.0	0.00	0.00	81.0	82.4
Cl_AAASAS_P_c2	7.34	8.95	0.0	0.0	1.01	1.68	14.7	4.9
Cl_AAASAS_M_c1	8.08	8.38	0.0	0.0	1.75	1.11	4.2	12.6
Cl_ASASAS_P_c1	10.15	11.26	0.0	0.0	0.00	0.00	98.3	99.3
Cl_ASASAS_M_c1	12.57	14.15	0.0	0.0	2.41	2.90	1.7	0.7

[a)] Referenced to E = -3322.321734 hartree and G = -3322.413149 hartree

Table S3. Key torsional angles of the optimized geometries of **1**·HCl. Angle definitions shown in Scheme S1.

	TREN head group				Thiourea moieties				α-methylbenzyl arms		
Conformer	**A1**	**A2**	**A3**		**B1**	**B2**	**B3**		**G1**	**G2**	**G3**
HCl_AAAAAA_P_c1	66.0	65.0	64.3	P	178.2	178.8	178.9	AA AA AA	27.8	28.6	27.5
HCl_AAAAAA_P_c2	64.5	65.4	65.1	P	-177.2	178.1	178.8	AA AA AA	-14.5	28.1	29.8
HCl_AAAAAA_P_c3	66.5	67.6	66.3	P	179.5	-176.4	-176.0	AA AA AA	30.9	-23.8	-24.3
HCl_AAAAAA_P_c4	68.8	67.9	68.3	P	-175.7	-176.1	-176.1	AA AA AA	-22.1	-22.7	-22.6
HCl_AAAAAA_P_c5	65.3	64.6	64.3	P	-177.1	-177.8	-176.2	AA AA AA	176.5	176.5	176.1
HCl_AAAAAA_M_c1	-65.5	-65.7	-66.0	M	177.0	176.2	176.1	AA AA AA	31.6	32.3	32.5
HCl_AAAAAA_M_c2	-65.0	-66.0	-65.4	M	176.4	176.8	178.6	AA AA AA	31.7	33.4	-16.2
HCl_AAAAAA_M_c3	-64.9	-66.3	-66.3	M	179.0	176.1	179.0	AA AA AA	-18.8	32.6	-20.9
HCl_AAAAAA_M_c4	-65.9	-65.7	-67.2	M	178.4	177.6	178.1	AA AA AA	-20.7	-15.1	-16.6
HCl_AAAAAA_M_c5	-64.9	-64.3	-65.2	M	179.6	179.0	179.2	AA AA AA	178.9	179.2	178.5
HCl_AAAAAA_PPL_c1	-65.5	72.6	70.3	M/PP	178.8	-179.9	177.2	AA AA AA	32.9	32.3	32.5
HCl_AAAAAA_PPL_c2	-65.5	66.3	70.5	M/PP	-178.2	179.9	-174.7	AA AA AA	176.3	177.9	175.6
HCl_AAAAAA_LLR_c1	65.6	-73.1	-67.9	P/MM	176.5	174.5	178.2	AA AA AA	31.1	32.5	34.0
HCl_AAAAAA_LLR_c2	66.0	-70.8	-69.4	P/MM	177.8	177.6	-178.7	AA AA AA	178.6	178.5	176.4
HCl_AAAAAS_P_c1	72.5	74.8	82.0	P	179.8	-179.2	-10.2	AA AA AS	31.4	31.7	48.9
HCl_AAAAAS_P_c2	72.4	75.3	82.4	P	-176.7	-179.9	-9.2	AA AA AS	-28.7	32.4	48.6
HCl_AAAAAS_P_c3	74.8	79.8	80.1	P	179.5	-175.9	-11.5	AA AA AS	32.9	-33.2	51.4
HCl_AAAAAS_P_c4	74.4	79.7	80.7	P	-177.0	-175.6	-11.4	AA AA AS	-28.0	-33.0	51.5
HCl_AAAAAS_M_c1	-73.7	-70.8	-83.2	M	175.0	176.3	10.1	AA AA AS	33.0	33.2	-43.1
HCl_AAAAAS_M_c2	-74.2	-71.6	-82.5	M	174.9	177.4	10.1	AA AA AS	33.0	-21.8	-42.5
HCl_AAAAAS_M_c3	-74.1	-70.6	-83.3	M	177.4	176.4	10.1	AA AA AS	-22.6	33.1	-43.1
HCl_AAAAAS_M_c4	-74.7	-71.5	-74.7	M	177.5	177.3	10.0	AA AA AS	-22.5	-22.0	-42.6
HCl_AAASAS_P_c1	77.6	82.9	82.2	P	179.0	-7.8	-9.0	AA AS AS	47.6	33.1	49.7
HCl_AAASAS_P_c2	80.1	81.5	81.8	P	-175.6	-11.4	-9.2	AA AS AS	-32.5	52.1	49.3
HCl_AAASAS_M_c1	-73.4	-83.0	-83.2	M	175.8	9.9	10.4	AA AS AS	35.1	-44.7	-45.2
HCl_AAASAS_M_c2	-73.6	-82.0	-83.2	M	176.6	9.7	10.6	AA AS AS	-21.8	-44.0	-45.3
HCl_ASASAS_P_c1	82.8	83.0	82.9	P	-9.5	-8.7	-8.6	AS AS AS	49.8	49.9	49.6
HCl_ASASAS_M_c1	-82.5	-83.0	-82.8	M	10.3	9.7	10.0	AS AS AS	-45.0	-44.7	-45.3

Table S4. Relative conformer energies (in kcal/mol) of **1**·HCl obtained considering all conformers together and sorted by individual conformer families.

	All conformers				Individual families			
Conformer	**ΔE_{ZPC}**	**ΔG_{298K}**	**$\chi(\Delta E)$**	**$\chi(\Delta G)$**	**ΔE_{ZPC}**	**ΔG_{298K}**	**$\chi(\Delta E)$**	**$\chi(\Delta G)$**
HCl_AAAAAA_P_c1	0.60	1.15	9.1	4.5	0.00	0.04	31.7	18.8
HCl_AAAAAA_P_c2	1.05	2.31	4.2	0.6	0.45	1.20	14.8	2.6
HCl_AAAAAA_P_c3	1.34	1.20	2.6	4.1	0.74	0.09	9.1	17.1
HCl_AAAAAA_P_c4	1.86	1.22	1.1	4.0	1.26	0.11	3.8	16.7
HCl_AAAAAA_P_c5	16.02	17.51	0.0	0.0	15.42	16.39	0.0	0.0
HCl_AAAAAA_M_c1	0.92	1.69	5.3	1.8	0.32	0.58	18.5	7.6
HCl_AAAAAA_M_c2	1.22	1.11	3.2	4.7	0.62	0.00	11.1	20.0
HCl_AAAAAA_M_c3	1.45	1.45	2.2	2.7	0.85	0.34	7.6	11.3
HCl_AAAAAA_M_c4	2.01	1.90	0.8	1.3	1.40	0.79	3.0	5.3
HCl_AAAAAA_M_c5	15.85	18.73	0.0	0.0	15.24	17.62	0.0	0.0
HCl_AAAAAA_PPM_c1	3.36	3.44	0.1	0.1	2.76	2.32	0.3	0.4
HCl_AAAAAA_PPM_c2	19.34	20.69	0.0	0.0	18.74	19.58	0.0	0.0
HCl_AAAAAA_MMR_c1	3.74	3.55	0.0	0.1	3.14	2.44	0.2	0.3
HCl_AAAAAA_MMR_c2	18.71	19.93	0.0	0.0	18.11	18.82	0.0	0.0
HCl_AAAAAS_P_c1	0.80	0.54	6.5	12.6	0.00	0.00	33.5	39.7
HCl_AAAAAS_P_c2	0.95	0.92	5.1	6.6	0.15	0.38	26.0	20.9
HCl_AAAAAS_P_c3	1.16	1.14	3.5	4.5	0.36	0.61	18.1	14.3
HCl_AAAAAS_P_c4	1.30	1.09	2.8	5.0	0.50	0.55	14.4	15.7
HCl_AAAAAS_M_c1	2.39	2.83	0.4	0.3	1.59	2.30	2.3	0.8
HCl_AAAAAS_M_c2	2.45	2.34	0.4	0.6	1.65	1.80	2.1	1.9
HCl_AAAAAS_M_c3	2.51	2.22	0.4	0.7	1.71	1.69	1.9	2.3
HCl_AAAAAS_M_c4	2.55	1.84	0.3	1.4	1.76	1.30	1.7	4.4
HCl_AAASAS_P_c1	0.15	**0.0**[a)]	19.4	31.1	0.00	0.00	72.6	88.2
HCl_AAASAS_P_c2	0.76	1.24	7.0	3.8	0.60	1.24	26.2	10.9
HCl_AAASAS_M_c1	2.91	3.28	0.2	0.1	2.76	3.28	0.7	0.3
HCl_AAASAS_M_c2	2.99	2.98	0.2	0.2	2.84	2.98	0.6	0.6
HCl_ASASAS_P_c1	**0.0**[a)]	0.72	25.1	9.2	0.00	0.00	99.6	99.4
HCl_ASASAS_M_c1	3.34	3.70	0.1	0.1	3.34	2.98	0.4	0.6

[a)] Referenced to E = -3322.761621 hartree and G = -3322.853482 hartree

Table S5. Key torsional angles of the optimized geometries of **1**·HSO_4^-. Angle definitions shown in Scheme S1.

	TREN head group				Thiourea moieties				α-methylbenzyl arms		
Conformer	**A1**	**A2**	**A3**		**B1**	**B2**	**B3**		**G1**	**G2**	**G3**
HSO4_AAAAAA_P_c1	70.3	73.0	71.4	**P**	173.4	176.3	178.7	AA AA AA	26.7	33.4	27.1
HSO4_AAAAAA_P_c2	71.0	72.7	71.8	**P**	176.0	-177.5	-178.2	AA AA AA	178.8	177.2	177.1
HSO4_AAAAAA_M_c1	-71.1	-73.5	-72.4	**M**	173.3	177.9	178.8	AA AA AA	21.7	32.6	26.1
HSO4_AAAAAA_M_c2	-70.8	-73.0	-72.0	**M**	-178.7	-180.0	177.4	AA AA AA	177.2	177.3	178.4
HSO4_AAAAAS_P_c1	75.0	76.0	84.0	**P**	-179.5	177.7	-15.2	AA AA AS	35.1	33.3	45.2
HSO4_AAAAAS_P_c2	69.2	86.2	73.0	**P**	170.2	-15.7	177.6	AA AA AS	23.1	42.5	30.0
HSO4_AAAAAS_P_c3	71.9	75.1	85.4	**P**	176.3	178.2	8.6	AA AA AS	30.0	34.0	-35.9
HSO4_AAAAAS_P_c4	74.8	76.3	83.0	**P**	-170.1	178.3	-17.6	AA AA AS	-26.6	31.3	52.7
HSO4_AAAAAS_M_c1	-87.1	-73.8	-76.6	**M**	-12.7	177.4	175.4	AA AA AS	48.5	31.8	31.2
HSO4_AAAAAS_M_c2	-74.1	-76.7	-85.0	**M**	176.9	176.5	15.0	AA AA AS	32.0	33.3	-42.9
HSO4_AAAAAS_M_c3	-84.0	-74.0	-76.2	**M**	12.2	177.2	176.9	AA AA AS	-36.8	31.7	31.5
HSO4_AAAAAS_M_c4	-83.7	-73.7	-75.8	**M**	12.1	-178.0	-179.5	AA AA AS	-36.5	-23.1	-16.0
HSO4_AAAAAS_M_c5	-72.9	-76.5	-85.3	**M**	-177.9	177.1	14.5	AA AA AS	-25.1	32.2	-42.3
HSO4_AAAAAS_M_c6	-69.9	-89.8	-72.8	**M**	-175.7	9.3	173.1	AA AA AS	5.4	-34.5	25.7
HSO4_AAAAAS_PPM_c1	-63.1	97.3	70.7	M/PP	172.1	-17.4	178.0	AA AA AS	29.2	44.8	31.2
HSO4_AAAAAS_MMP_c1	68.2	-101.4	-66.0	P/MM	178.5	18.5	173.4	AA AA AS	30.0	-45.4	27.4

Table S6. Relative conformer energies (in kcal/mol) of **1**·HSO_4^- obtained considering all conformers together and sorted by individual conformer families.

	All conformers				Individual families			
Conformer	**ΔE_{ZPC}**	**ΔG_{298K}**	**χ(ΔE)**	**χ(ΔG)**	**ΔE_{ZPC}**	**ΔG_{298K}**	**χ(ΔE)**	**χ(ΔG)**
HSO4_AAAAAA_R_c1	**0.0**[a)]	0.50	62.3	30.0				
HSO4_AAAAAA_L_c1	0.33	**0.0**[a)]	35.9	69.5				
HSO4_AAAAAA_R_c2	15.03	15.47	0.0	0.0				
HSO4_AAAAAA_L_c2	15.20	15.95	0.0	0.0				
HSO4_AAAAAS_R_c1	2.67	4.18	0.7	0.1	0.00	0.91	39.5	11.6
HSO4_AAAAAS_R_c2	3.40	4.48	0.2	0.0	0.73	1.21	11.4	6.9
HSO4_AAAAAS_R_c3	3.62	5.22	0.1	0.0	0.95	1.94	7.9	2.0
HSO4_AAAAAS_R_c4	3.67	5.15	0.1	0.0	1.01	1.88	7.2	2.2
HSO4_AAAAAS_L_c1	3.09	4.00	0.3	0.1	0.42	0.73	19.3	15.7
HSO4_AAAAAS_L_c2	3.73	3.27	0.1	0.3	1.07	0.00	6.5	53.5
HSO4_AAAAAS_L_c3	3.86	4.73	0.1	0.0	1.20	1.46	5.2	4.6
HSO4_AAAAAS_L_c4	4.78	5.07	0.0	0.0	2.11	1.80	1.1	2.6
HSO4_AAAAAS_L_c5	4.90	6.37	0.0	0.0	2.24	3.10	0.9	0.3
HSO4_AAAAAS_L_c6	4.95	5.99	0.0	0.0	2.29	2.72	0.8	0.5
HSO4_AAAAAS_PPM_c1	6.64	7.17	0.0	0.0	3.97	3.90	0.0	0.1
HSO4_AAAAAS_MMP_c1	7.76	8.31	0.0	0.0	5.10	5.04	0.0	0.0

[a)] Referenced to E = -3561.891647 hartree and G = -3561.983777 hartree

Table S7. Comparison of the relative energies and populations obtained with different dispersion-corrected functionals. ΔG_{corr} corresponds to the Gibbs free energies obtained after entropic correction (J. Phys. Chem. B 2011, **115**, 14556)

		Relative energies in kcal/mol				**Boltzmann populations in %**		
	Conformer	**ΔE_{elec}**	**ΔE_{ZPC}**	**ΔG_{298K}**	**ΔGcorr**	**$\chi(\Delta E_{elec})$**	**$\chi(\Delta E_{ZPC})$**	**$\chi(\Delta G_{298K})$**
B3LYP	Cl_AAAAAA_P_c1	0.00	0.00	0.35	0.00	58.0	55.1	35.8
	Cl_AAAAAA_M_c1	0.19	0.12	0.00	0.07	41.9	44.8	64.1
	Cl_AAAAAS_P_c1	4.15	4.28	4.28	4.29	0.1	0.0	0.0
	Cl_AAAAAS_M_c1	3.97	4.11	4.27	4.11	0.1	0.1	0.0
B3LYP-GD3BJ	Cl_AAAAAA_P_c1	0.00	0.00	0.00		99.8	99.8	98.8
	Cl_AAAAAA_M_c1	8.31	7.48	2.93		0.0	0.0	0.7
	Cl_AAAAAS_P_c1	3.70	3.73	3.17		0.2	0.2	0.5
	Cl_AAAAAS_M_c1	7.69	7.33	6.24		0.0	0.0	0.0
wB97XD	Cl_AAAAAA_P_c1	0.00	0.00	0.00		100.0	100.0	99.8
	Cl_AAAAAA_M_c1	8.41	7.71	3.85		0.0	0.0	0.1
	Cl_AAAAAS_P_c1	7.53	6.90	6.48		0.0	0.0	0.0
	Cl_AAAAAS_M_c1	7.45	7.12	6.51		0.0	0.0	0.0
M06-2X	Cl_AAAAAA_P_c1	0.00	0.00	0.00		100.0	100.0	99.2
	Cl_AAAAAA_M_c1	7.60	6.82	2.87		0.0	0.0	0.8
	Cl_AAAAAS_P_c1	6.84	6.56	5.53		0.0	0.0	0.0
	Cl_AAAAAS_M_c1	7.27	6.96	6.30		0.0	0.0	0.0

4. Computed IR and VCD spectra

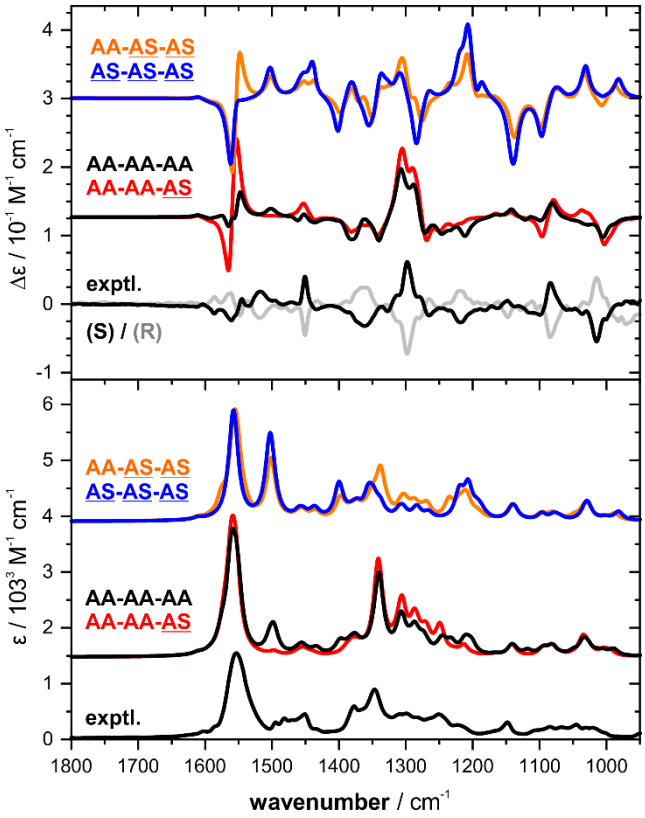


Figure S1. Conformer family spectra of **1**·Cl^-

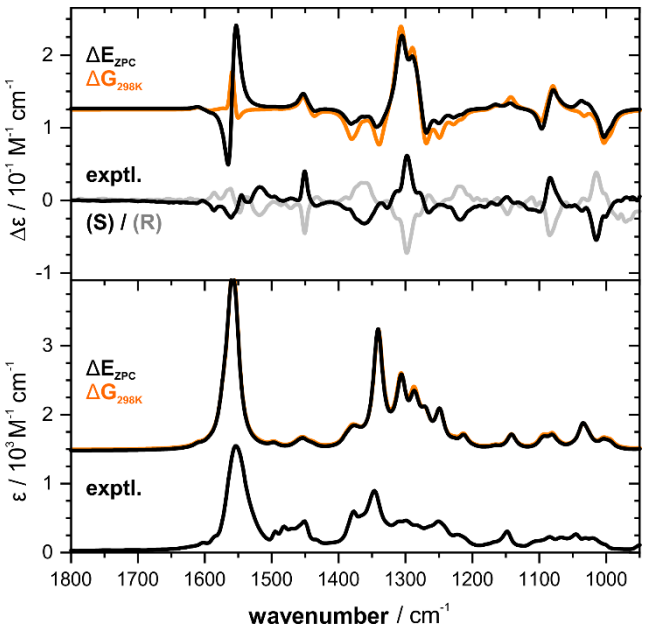


Figure S2. ΔE_{ZPC}- and ΔG_{298K}-weighted spectra of **1**·Cl^-

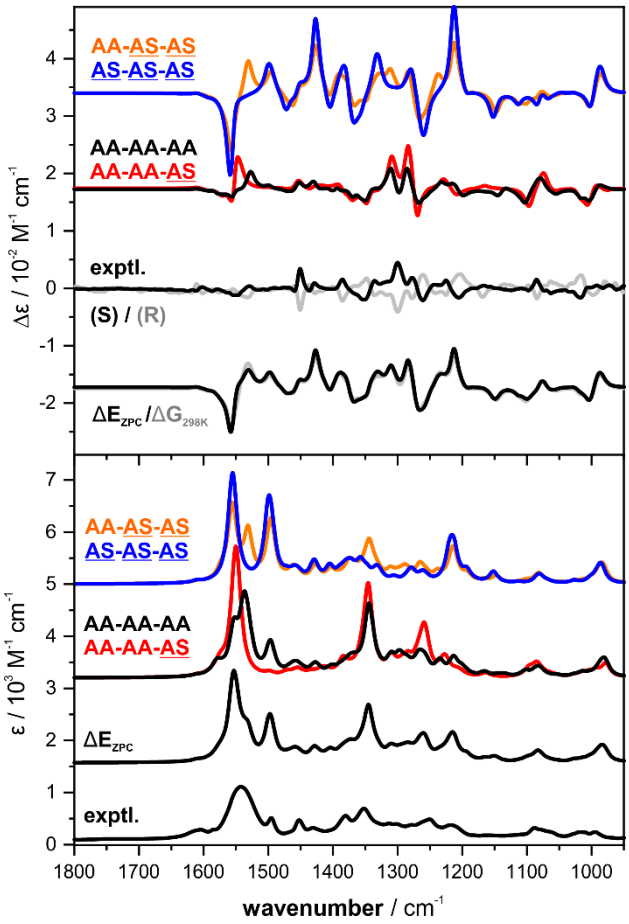


Figure S3. Conformer family spectra of **1**·HCl

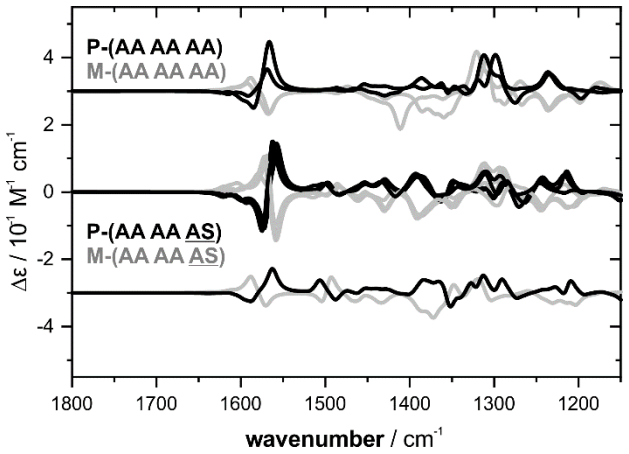


Figure S4. Single-conformer spectra of **1**·HSO_4^-

5. Cartesian coordinates

Cl_AAAAAA_M_c1

Charge: -1 Multiplicity: 1

N	-0.48343000	-0.09065900	3.88969400
C	-0.35365000	1.28380100	4.38935600
H	0.70474000	1.49945000	4.55921900
H	-0.86241800	1.40443200	5.36383500
C	-1.83589400	-0.62651800	4.08864900
H	-2.55455600	0.19513800	4.02808700
H	-1.94568100	-1.06970100	5.09578200
C	0.54858400	-0.97870500	4.43882100
H	0.20998200	-2.01402500	4.34260500
H	0.70109700	-0.79378100	5.51853700
C	-0.89457200	2.33590600	3.41538700
H	-0.84642300	3.31977000	3.88402900
H	-1.94246300	2.13182800	3.16948300
C	-2.23436300	-1.67151500	3.04002400
H	-3.20535500	-2.09358800	3.30355600
H	-1.50755300	-2.49029700	3.01409600
C	1.89759700	-0.85902200	3.72160400
H	2.63628100	-1.47304400	4.23838300
H	2.25299100	0.17708500	3.73651200
N	-0.14183400	2.39313700	2.17480400
H	-0.23614800	1.59565800	1.54906800
N	-2.32875300	-1.11807500	1.70048500
H	-1.44883800	-0.88715200	1.24297300
N	1.84008000	-1.29724300	2.33837800
H	1.31331700	-0.70772700	1.69690400
C	0.77213900	3.33000200	1.83432400
C	-3.45920700	-0.69275300	1.09112500
C	2.28377100	-2.47962400	1.85441400
S	1.11260300	4.69836200	2.79858400
S	-5.01759700	-0.91143500	1.75471500
S	3.12514400	-3.62221200	2.80624700
N	1.40066700	3.08988200	0.65875300
H	1.15216700	2.22900600	0.17246700
N	-3.25059900	-0.07697600	-0.09690300
H	-2.28099300	0.03974800	-0.38936500
N	2.00152600	-2.68351700	0.54544900
H	1.46661600	-1.95537900	0.07286700
C	2.37350000	3.96198100	0.01347200
H	2.90881900	4.48380600	0.80999000
C	-4.28400600	0.41763700	-0.99809200
H	-5.12571900	0.72858300	-0.37483200
C	2.42112200	-3.82767000	-0.25390500
H	2.49831500	-4.67726500	0.42828700
Cl	0.15544400	0.05937800	-0.32702000
C	3.78461700	-3.63698600	-0.91482300
C	4.62545000	-4.74198100	-1.08869000
C	4.20198000	-2.39443200	-1.40383200
C	5.85354700	-4.61356500	-1.73905400
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C	5.43020500	-2.26039300	-2.05370100
H	3.57079200	-1.52160900	-1.26902900
C	6.26029600	-3.36968900	-2.22548700
H	6.49501400	-5.48174500	-1.85665100
H	5.73904800	-1.28715000	-2.42302100
H	7.21736600	-3.26443600	-2.72686800
C	1.73709300	5.01753900	-0.88819700

C	2.35215100	6.26712300	-1.02437400
C	0.58093700	4.75577500	-1.63078800
C	1.82979000	7.23354700	-1.88494800
H	3.24290900	6.48984500	-0.44268100
C	0.05333700	5.71985800	-2.49174000
H	0.08103000	3.79747000	-1.53032900
C	0.67668300	6.96194100	-2.62396300
H	2.31772900	8.19978900	-1.97081800
H	-0.84709100	5.49986800	-3.05730400
H	0.26423600	7.71299300	-3.29049000
C	-4.79290600	-0.64107800	-1.97320700
C	-6.14127100	-0.64463400	-2.34654200
C	-3.93499300	-1.58250000	-2.55216700
C	-6.62445900	-1.56304700	-3.27991000
H	-6.82237300	0.07100100	-1.89357800
C	-4.41357900	-2.50446500	-3.48456400
H	-2.88767200	-1.60485400	-2.26714700
C	-5.76015600	-2.49728800	-3.85363300
H	-7.67598300	-1.55437800	-3.55058300
H	-3.73358700	-3.23037900	-3.92010900
H	-6.13336900	-3.21695000	-4.57561300
C	1.33571600	-4.12527900	-1.30160700
H	0.37955300	-4.33613100	-0.81248000
H	1.20049900	-3.27655700	-1.98124800
H	1.62211000	-4.99334400	-1.90155600
C	-3.73879600	1.64307000	-1.74957800
H	-3.44699700	2.42718900	-1.04393700
H	-2.86631500	1.37650400	-2.35655800
H	-4.50492800	2.04165000	-2.42009100
C	3.36933500	3.09392100	-0.77343400
H	3.87615200	2.39063300	-0.10527200
H	2.85934100	2.52466200	-1.55853700
H	4.12105600	3.72708100	-1.25238200

Cl_AAAAAA_P_c1

Charge: -1 Multiplicity: 1

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H	1.50618400	1.32452700	3.62585000
C	-0.96659100	1.51832300	3.45857000
H	-0.76885900	1.89118100	4.48078300
H	-2.04149000	1.32851400	3.39519200
C	-0.98866100	-0.90239100	3.71573000
H	-1.42062400	-0.69454100	4.71231600
H	-0.29151200	-1.73494200	3.84232600
C	2.08916300	-0.63004700	2.99217200
H	1.73801300	-1.66737500	3.03995200
H	3.06719000	-0.58856900	3.47325700
C	-0.62856800	2.62623400	2.45556500
H	0.44933000	2.82295500	2.44278100
H	-1.13084000	3.54735300	2.75389800
C	-2.10841300	-1.37083600	2.78060100
H	-2.81589500	-0.55765400	2.58383300
H	-2.65878600	-2.18264600	3.25797200
N	2.26249200	-0.26059200	1.59870000
H	1.43803200	-0.33056400	1.00582900
N	-1.05318700	2.30232000	1.10541000
H	-0.57344700	1.52639900	0.65328200
N	-1.60578700	-1.85731100	1.50817900
H	-1.18982400	-1.16343900	0.89000300

C	3.38894700	0.22061100	1.02564200
C	-2.08936500	2.85353900	0.43367500
C	-1.53400400	-3.14814900	1.11101600
S	4.84599200	0.46745400	1.88258500
S	-3.05697200	4.10964400	1.06980700
S	-2.10093100	-4.45237400	2.05758500
N	3.26952200	0.47775700	-0.29884900
H	2.35781300	0.30175900	-0.72027200
N	-2.28364000	2.33766700	-0.80362700
H	-1.65977500	1.58297800	-1.08805300
N	-0.98987200	-3.31756700	-0.11801900
H	-0.67066000	-2.47583500	-0.59666900
C	4.29184300	1.07038200	-1.15249200
H	5.25817300	0.73103500	-0.77294600
C	-3.37002700	2.68064500	-1.71391600
H	-3.61646100	3.72850800	-1.52984800
C	-0.73710700	-4.59126000	-0.78010900
H	-1.51233400	-5.28326200	-0.44396900
C	4.29139900	2.59726000	-1.12707500
C	5.50210900	3.28935100	-1.24118900
C	3.10448900	3.33352800	-1.04485300
C	5.53018400	4.68434300	-1.27592700
H	6.43339600	2.73114800	-1.29055000
C	3.12722700	4.72889300	-1.07612700
H	2.15426000	2.81780900	-0.94658600
C	4.34030800	5.40997400	-1.19360000
H	6.48088600	5.20275600	-1.35675000
H	2.19597000	5.28270000	-1.00610100
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C	-4.57845500	0.48965800	-1.18444900
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C	-5.74894500	-0.25383100	-1.02589100
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C	-7.06203200	1.72266500	-1.45795000
H	-5.94668400	3.52601200	-1.82739400
C	-6.99575600	0.35962400	-1.16426600
H	-5.68539300	-1.31203300	-0.79152300
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C	0.74794800	-6.59300500	-0.35862300
C	1.75325100	-4.41166800	-0.21788500
C	1.98319400	-7.18543900	-0.09242000
H	-0.12855100	-7.21908900	-0.50408600
C	2.99072500	-4.99902100	0.05140800
H	1.67369600	-3.32972900	-0.25529500
C	3.11102700	-6.38857700	0.11313000
H	2.06177600	-8.26699800	-0.03617700
H	3.85943400	-4.36900500	0.21605000
H	4.07237700	-6.84522400	0.32685500
C	4.10425200	0.54203100	-2.58417300
H	4.17969800	-0.54979500	-2.60260600
H	3.12656300	0.83119900	-2.98550000
H	4.87317900	0.95848300	-3.24046500
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H	-2.57499700	1.49827600	-3.37169900
H	-3.66439500	2.80421200	-3.86037400
C	-0.87152500	-4.39133700	-2.29898400
H	-1.87197200	-4.02496400	-2.54996700

H	-0.13312200	-3.67060500	-2.66766600
H	-0.70385200	-5.33890300	-2.81810200
Cl	0.00340200	-0.17938800	-0.99750200

Cl_AAAAAS_M_c1

Charge: -1 Multiplicity: 1

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H	-2.36195000	0.18070900	4.01939600
H	-1.64085500	-1.17043900	4.89696700
C	0.81408200	-0.89245400	4.06134200
H	0.48572300	-1.93165700	3.98834200
H	1.12852300	-0.74113000	5.10895800
C	-0.82256600	2.45693900	3.61160200
H	-0.78280000	3.36443800	4.21540300
H	-1.87645800	2.23806800	3.40566500
C	-2.03470400	-1.54815400	2.80496000
H	-2.99373400	-2.00818200	3.04695900
H	-1.30016700	-2.35062100	2.67469200
C	2.03717700	-0.71701900	3.14740600
H	2.92719200	-1.09027600	3.65629100
H	2.18949900	0.34171300	2.92007000
N	-0.15311100	2.72737500	2.35258400
H	-0.18630700	1.98519000	1.65378000
N	-2.17224300	-0.84985400	1.53882400
H	-1.31302200	-0.46987900	1.14390600
N	1.92294600	-1.41882200	1.87120300
H	1.49366200	-0.89569400	1.11005400
C	0.65033200	3.77980000	2.08221900
C	-3.32997400	-0.44760100	0.96640600
C	2.29051200	-2.70016500	1.68563800
S	0.88760400	5.08293000	3.16371800
S	-4.86993500	-0.89946900	1.55510600
S	2.95183000	-3.67514100	2.93454600
N	1.26129700	3.71299600	0.87498300
H	1.07476400	2.88069800	0.31531600
N	-3.16294600	0.34728200	-0.11701200
H	-2.20180600	0.57567100	-0.37219800
N	2.12887000	-3.25234300	0.46096600
H	2.44821200	-4.20876000	0.40831600
C	2.09110000	4.75092100	0.27596900
H	2.56885500	5.28549600	1.09986600
C	-4.22113700	0.85221800	-0.98542200
H	-5.12432500	0.90872100	-0.37505200
C	1.74574200	-2.60175700	-0.80525000
H	0.97639000	-1.85747900	-0.58631100
Cl	0.21724400	0.71685100	-0.32113300
C	1.11258600	-3.65105300	-1.70834500
C	-0.27144200	-3.65067300	-1.91435500
C	1.88257300	-4.64418300	-2.32825000
C	-0.87549100	-4.61641700	-2.72098100
H	-0.88221900	-2.88909100	-1.43924600
C	1.28177400	-5.61495900	-3.13099200
H	2.95943200	-4.66643700	-2.18983100
C	-0.09989000	-5.60320200	-3.33099000
H	-1.95072100	-4.59709400	-2.86764200
H	1.89411200	-6.37800100	-3.60152700
H	-0.56730500	-6.35666300	-3.95714400

C	1.29065900	5.76635400	-0.53634900
C	1.63667400	7.12077300	-0.48740700
C	0.24176900	5.37276900	-1.37548200
C	0.95684700	8.06339800	-1.26096200
H	2.43906500	7.44284100	0.17097000
C	-0.44241000	6.31133000	-2.14907500
H	-0.05183500	4.32833800	-1.41993600
C	-0.08612200	7.66063900	-2.09653400
H	1.23594500	9.11115700	-1.20283600
H	-1.25560300	5.98796600	-2.79182500
H	-0.62104200	8.39115300	-2.69544800
C	-4.51179400	-0.07021900	-2.16610100
C	-5.83394700	-0.37238600	-2.50627400
C	-3.48001800	-0.59307900	-2.95544600
C	-6.12439200	-1.17537400	-3.61155200
H	-6.64393200	0.01660200	-1.89555400
C	-3.76453100	-1.39759500	-4.05912700
H	-2.44527700	-0.37775900	-2.70519000
C	-5.08917400	-1.69080500	-4.39237100
H	-7.15750700	-1.40373200	-3.85554100
H	-2.95125200	-1.79515900	-4.65860800
H	-5.31080300	-2.31875100	-5.24976400
C	2.93808800	-1.87717700	-1.45106900
H	3.33024700	-1.11230700	-0.77481000
H	3.74921400	-2.57262500	-1.68636700
H	2.62056700	-1.38361300	-2.37447900
C	-3.84744000	2.26555100	-1.45887700
H	-3.71472000	2.93298600	-0.60188300
H	-2.91787200	2.25547200	-2.03869700
H	-4.63815000	2.66721200	-2.09885700
C	3.17671500	4.08476900	-0.58470500
H	3.79151800	3.41577500	0.02567800
H	2.73250500	3.50271800	-1.39988200
H	3.82223800	4.84715400	-1.02957300

Cl_AAAAAS_P_c1

Charge: -1 Multiplicity: 1

N	-0.19416900	0.13693600	3.22502600
C	1.14724700	0.26421500	3.80658300
H	1.18458600	-0.14735800	4.83226000
H	1.39215400	1.32725100	3.88172000
C	-1.09159300	1.21166700	3.67449500
H	-0.98434900	1.38472700	4.76168000
H	-2.12452700	0.89254300	3.50721100
C	-0.79275900	-1.18462900	3.46452600
H	-1.35485400	-1.18964400	4.41499600
H	-0.00199500	-1.93076500	3.57158700
C	2.23454900	-0.40901000	2.96580700
H	2.06254200	-1.49147000	2.90362600
H	3.20626600	-0.25892300	3.43785300
C	-0.89298000	2.54082700	2.94263400
H	0.14487400	2.88514300	3.03140000
H	-1.53077400	3.30050000	3.39660200
C	-1.72527900	-1.63929200	2.33126400
H	-2.29128200	-0.78724800	1.94409200
H	-2.43250600	-2.37531900	2.71483100
N	2.29372100	0.14850200	1.62708100
H	1.41968200	0.14613600	1.10400100
N	-1.24824700	2.44439300	1.53923400
H	-0.75445000	1.73857700	0.99317500
N	-1.02319400	-2.24234700	1.20132100

H	-0.70048600	-1.59507900	0.48356300
C	3.37922400	0.66923100	1.01202300
C	-2.19260500	3.16496400	0.89495400
C	-0.83076700	-3.56594700	1.05665400
S	4.90844300	0.80530800	1.76340900
S	-3.16477000	4.34267300	1.66579000
S	-1.33549500	-4.71909100	2.22635400
N	3.15420600	1.06469000	-0.26303900
H	2.21242100	0.92021800	-0.62926900
N	-2.29297500	2.88442100	-0.42631500
H	-1.67203600	2.15776500	-0.78398900
N	-0.22370700	-4.02256400	-0.06307200
H	-0.10166300	-5.02499300	-0.06509100
C	4.10455500	1.75434800	-1.12633500
H	5.09999800	1.40023100	-0.84897000
C	-3.28671500	3.42152800	-1.34683600
H	-3.57113800	4.40284100	-0.96184000
C	0.40056500	-3.26954600	-1.16352500
H	-0.09287400	-2.29870800	-1.23349300
C	4.08415400	3.27111700	-0.95227500
C	5.27648100	3.99475700	-1.06150400
C	2.89255600	3.97215600	-0.73618800
C	5.28221800	5.38698600	-0.96123700
H	6.21157200	3.46260000	-1.21553900
C	2.89307200	5.36405900	-0.63226500
H	1.95700000	3.43013100	-0.63869100
C	4.08799100	6.07734100	-0.74643100
H	6.21937900	5.92969000	-1.04090100
H	1.95906200	5.88982200	-0.45898700
H	4.08900000	7.15957000	-0.66120200
C	-4.55019600	2.56786800	-1.43190600
C	-4.49723000	1.16911600	-1.41809100
C	-5.79514900	3.18916900	-1.57870700
C	-5.66145100	0.41062300	-1.54996700
H	-3.54347100	0.66490900	-1.29501400
C	-6.96216400	2.43499200	-1.71301700
H	-5.85308300	4.27443600	-1.57741500
C	-6.89867600	1.04060900	-1.69972300
H	-5.60098400	-0.67336000	-1.53280500
H	-7.91945800	2.93659200	-1.81826800
H	-7.80445600	0.45039100	-1.79800000
C	0.14768700	-3.99884900	-2.47616800
C	-0.66462900	-3.41629600	-3.45492200
C	0.71334000	-5.25464900	-2.73486300
C	-0.91028900	-4.07083000	-4.66352100
H	-1.10545700	-2.44099200	-3.27123900
C	0.46403700	-5.91542700	-3.93801800
H	1.35776900	-5.72671200	-1.99848000
C	-0.34858600	-5.32438700	-4.90775000
H	-1.54122400	-3.60041700	-5.41124800
H	0.90827000	-6.88928500	-4.11901500
H	-0.53981300	-5.83627200	-5.84561600
C	3.82259100	1.36074800	-2.58558500
H	3.91500700	0.27769600	-2.71400300
H	2.81343300	1.66231300	-2.88734800
H	4.53496200	1.85558400	-3.25136600
C	-2.64141600	3.59564200	-2.73179600
H	-1.78202700	4.27068600	-2.67010200
H	-2.30088800	2.63414000	-3.13192900
H	-3.36756000	4.01378000	-3.43463700
C	1.89461200	-3.02834600	-0.89219400

H	2.02806900	-2.46515300	0.03558100
H	2.43896700	-3.97340200	-0.80047900
H	2.33738500	-2.45164300	-1.70971500
Cl	-0.10385700	0.36621400	-0.85514100

HCl_AAAAAA_M_c1

Charge: 0 Multiplicity: 1

N	-0.45906800	0.04540100	3.37041000
C	-0.79353900	1.46354700	3.79248600
H	0.14429000	1.98079700	3.99414200
H	-1.36372200	1.39449000	4.72104900
C	-1.60326600	-0.91435900	3.63535900
H	-2.53321100	-0.35031400	3.56444200
H	-1.48582200	-1.27380100	4.65961900
C	0.84508900	-0.43469600	3.97750400
H	0.82253000	-1.52412500	3.99993600
H	0.87378700	-0.06119100	5.00293800
C	-1.56235700	2.22603200	2.71043400
H	-1.85182300	3.18805000	3.13865800
H	-2.47689800	1.70068400	2.42244900
C	-1.64163100	-2.06928900	2.63099700
H	-2.42178700	-2.75709500	2.96378100
H	-0.69757400	-2.62037500	2.61529700
C	2.06307600	0.02754900	3.17288900
H	2.95135200	-0.25826900	3.74007500
H	2.07691400	1.11485300	3.05715900
N	-0.77331400	2.44632900	1.51578200
H	-0.85827600	1.77613100	0.75379900
N	-1.93243700	-1.62935300	1.28188100
H	-1.15000200	-1.43169300	0.66125800
N	2.12244500	-0.56587500	1.85285300
H	1.71284600	-0.05045600	1.07629000
C	0.14146400	3.44767200	1.36127600
C	-3.18494600	-1.39022300	0.79426200
C	2.61863100	-1.80769400	1.57862900
S	0.37977100	4.64423700	2.54192000
S	-4.58386800	-1.68739600	1.70946600
S	3.34509400	-2.77494000	2.76997800
N	0.83230800	3.38777700	0.20406000
H	0.68226600	2.56867300	-0.38145500
N	-3.20137900	-0.89299600	-0.45961200
H	-2.30312900	-0.64873400	-0.87157300
N	2.46930100	-2.18810500	0.29295000
H	1.92401800	-1.57542700	-0.31029500
C	1.82556800	4.36072600	-0.24961200
H	2.30839900	4.75975000	0.64566900
C	-4.39863000	-0.61970800	-1.25413000
H	-5.18255800	-0.32448900	-0.55262600
C	2.97680700	-3.42743100	-0.29431300
H	2.94539200	-4.18587100	0.49164200
Cl	0.10055500	0.12578700	-0.71035000
C	4.42040100	-3.31107500	-0.77452200
C	4.89407900	-2.15870700	-1.41103300
C	5.28452100	-4.40122500	-0.62884400
C	6.20249900	-2.09825600	-1.89285800
H	4.24274700	-1.29759000	-1.52585700
C	6.59297600	-4.34648900	-1.11145000

H	4.93400000	-5.29781700	-0.12472800
C	7.05648800	-3.19307800	-1.74631200
H	6.55461000	-1.19491400	-2.38143600
H	7.25082800	-5.20052800	-0.98339300
H	8.07502500	-3.14537500	-2.11827100
C	1.21001300	5.53161400	-1.00984600
C	1.73485700	6.81652400	-0.83730900
C	0.16491600	5.34952000	-1.92212300
C	1.23174900	7.89807600	-1.56200800
H	2.53776200	6.97462700	-0.12234200
C	-0.34344500	6.42844600	-2.64680000
H	-0.26300900	4.36185300	-2.06494200
C	0.18949400	7.70687500	-2.47047900
H	1.64784300	8.88915100	-1.40978300
H	-1.15694200	6.26988300	-3.34807900
H	-0.20762000	8.54670200	-3.03176700
C	-4.89397600	-1.84187500	-2.02160800
C	-6.26813900	-2.07738500	-2.13127500
C	-4.00935100	-2.71141400	-2.66923400
C	-6.75230200	-3.15484600	-2.87500300
H	-6.96586300	-1.41782400	-1.62247200
C	-4.48850900	-3.79166500	-3.41143600
H	-2.93816900	-2.55211100	-2.58959300
C	-5.86252100	-4.01635900	-3.51835400
H	-7.82230300	-3.32500900	-2.94343100
H	-3.78801900	-4.45832400	-3.90498400
H	-6.23543400	-4.85813000	-4.09317700
C	2.04023200	-3.85148200	-1.43592100
H	1.02134100	-4.00101500	-1.06494900
H	2.01792400	-3.09701500	-2.23014300
H	2.39227600	-4.78833000	-1.87498600
C	-4.10520200	0.55500600	-2.19951400
H	-3.82136700	1.44669400	-1.63162200
H	-3.29561500	0.31011400	-2.89608700
H	-4.99543200	0.78620100	-2.78983400
C	2.87550300	3.63078100	-1.10118700
H	3.36498700	2.84279900	-0.52012400
H	2.41950800	3.18019200	-1.98978000
H	3.63655200	4.33885400	-1.43853700
H	-0.31985600	0.06488300	2.35080600

HCl_AAAAAA_P_c1

Charge: 0 Multiplicity: 1

C	0.16705100	1.42790300	3.23440200
N	-0.00441100	-0.02016800	2.81927700
C	1.15927900	-0.88661800	3.25929400
H	0.92152600	-1.25931100	4.25744000
C	1.42740200	-2.02726700	2.27439800
N	1.86039900	-1.54494400	0.97800900
C	3.14771800	-1.22094700	0.65666000
N	3.30460600	-0.78020900	-0.60827900
H	2.45681700	-0.63549300	-1.15368600
C	4.56422000	-0.34185100	-1.21377800
C	4.82455300	1.14906600	-1.02184700
C	6.07280500	1.58528000	-0.56712700
C	6.34805200	2.94742800	-0.42841200
C	5.37142900	3.89358700	-0.74063100
C	4.12041300	3.46823600	-1.19368100
C	3.85170900	2.10664500	-1.33544400
H	2.87436300	1.79213400	-1.69067200
H	3.35377100	4.19682300	-1.43839900

H	5.58041800	4.95285800	-0.62976400
H	7.32189400	3.26641700	-0.07006000
H	6.83355400	0.85330100	-0.31138800
C	4.56051300	-0.73215400	-2.69908000
H	5.50249200	-0.43069800	-3.16497800
H	4.44401400	-1.81454700	-2.81077400
H	3.74638100	-0.23552500	-3.23855400
H	5.35728000	-0.89072300	-0.70326400
S	4.42106200	-1.38079500	1.76887700
H	1.16231900	-1.44849600	0.24375400
H	0.54040700	-2.64958600	2.12825300
H	2.20627600	-2.65593900	2.71047500
H	2.04369400	-0.25274700	3.32124800
C	-1.33952600	-0.58827800	3.25876600
H	-1.53988600	-0.19531500	4.25740300
C	-2.46084500	-0.24603000	2.27501700
N	-2.25380100	-0.85080300	0.97449600
C	-2.64336600	-2.11430700	0.63164700
N	-2.34217600	-2.45607800	-0.63757300
C	-2.61820100	-3.74944800	-1.26676300
C	-1.46908500	-4.74025700	-1.10819300
C	-1.73006900	-6.04692000	-0.68416400
C	-0.69981900	-6.98366700	-0.57627700
C	0.61064500	-6.62102700	-0.88879900
C	0.88227500	-5.31766200	-1.31153900
C	-0.15071100	-4.38654800	-1.42249700
H	0.07711700	-3.37751800	-1.75468800
H	1.89874900	-5.02614500	-1.55718500
H	1.41436300	-7.34527400	-0.80206500
H	-0.92173300	-7.99228100	-0.24164800
H	-2.74651400	-6.33259000	-0.42891500
C	-2.96919200	-3.51660100	-2.74373300
H	-3.19876900	-4.47046100	-3.22624600
H	-2.13207900	-3.06101100	-3.28424400
H	-3.84024100	-2.85995000	-2.83160000
H	-3.48971600	-4.15916100	-0.75363900
H	-1.77541200	-1.79754600	-1.16899500
S	-3.44493300	-3.13789400	1.72424700
H	-1.81076500	-0.29206600	0.24869000
H	-3.39354100	-0.61609600	2.70512900
H	-2.56161800	0.83411500	2.13939500
H	-1.23602200	-1.67165500	3.31957800
H	0.59410500	1.42229600	4.23902500
C	1.04044000	2.21112800	2.25100300
N	0.42311000	2.34946400	0.94762100
C	-0.46785600	3.32537000	0.60522400
N	-0.91656300	3.23621300	-0.66393400
C	-1.90239700	4.11853300	-1.29147300
C	-3.33354400	3.61594500	-1.12657800
C	-4.33810600	4.49749000	-0.71550100
C	-5.66305200	4.07056700	-0.60272800
C	-5.99956300	2.74912900	-0.89788300
C	-5.00327900	1.86011900	-1.30808600
C	-3.68178700	2.29220000	-1.42377900
H	-2.91906300	1.58873100	-1.74592100
H	-5.25527100	0.82997000	-1.54007400
H	-7.02752200	2.41282600	-0.80721500
H	-6.42815100	4.76887700	-0.27791100
H	-4.08110900	5.52490400	-0.47385200
C	-1.53210600	4.30177100	-2.77083300
H	-0.52864800	4.72824400	-2.86473300

H	-2.24611000	4.97534100	-3.25235300
H	-1.55810000	3.34708600	-3.30807000
H	-1.82129600	5.08005800	-0.78188300
H	-0.63337000	2.41397700	-1.19369400
S	-0.94081900	4.53869200	1.69563400
H	0.66097500	1.66941600	0.22839100
H	1.20521600	3.20043900	2.68212300
H	2.01794700	1.73951300	2.11862000
H	-0.82285300	1.88203900	3.27479400
Cl	0.00922900	-0.02887700	-1.37071400
H	-0.00487300	-0.03412500	1.79003600

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Charge: 0 Multiplicity: 1

N	-0.56845900	0.08678800	3.24182600
C	-0.53525200	1.48202900	3.84116200
H	0.50976400	1.75816100	3.98398200
H	-1.00943300	1.40394500	4.82223900
C	-1.90967800	-0.57669700	3.49380200
H	-2.67651100	0.19718200	3.46717000
H	-1.86368500	-0.98493800	4.50597800
C	0.56500100	-0.75781100	3.79531000
H	0.28082400	-1.80579000	3.71034900
H	0.63582000	-0.50966200	4.85629600
C	-1.22133700	2.54517900	2.97897500
H	-1.35290600	3.42955100	3.60466500
H	-2.21334600	2.21940200	2.65322700
C	-2.26210600	-1.66497200	2.47684400
H	-3.13261500	-2.19592200	2.86630300
H	-1.45200000	-2.39192400	2.36805700
C	1.90555400	-0.53669100	3.08520600
H	2.69291200	-0.83338800	3.77918700
H	2.05945100	0.51826700	2.84066300
N	-0.45820800	2.91359200	1.80505900
H	-0.50990900	2.26621500	1.01798500
N	-2.57735600	-1.14405600	1.16319200
H	-1.77966800	-0.92050500	0.56765400
N	2.05625300	-1.30310000	1.86166800
H	1.69539900	-0.86462300	1.01714700
C	0.58522600	3.78891600	1.80927600
C	-3.77789900	-0.60463800	0.81417300
C	2.44221600	-2.60059200	1.83334200
S	0.93877700	4.79008800	3.13404800
S	-5.15634700	-0.71909100	1.79817200
S	2.80286400	-3.48540800	3.24878500
N	1.30652000	3.78726000	0.66582600
H	1.06419800	3.09260700	-0.03232800
N	-3.76949500	0.02557400	-0.38190900
H	-2.87583900	0.11012400	-0.85369200
N	2.53112100	-3.20077000	0.62770700
H	2.83528900	-4.16290300	0.67473100
C	2.41234700	4.68862600	0.34440200
H	2.92127900	4.90853100	1.28569100
C	-4.92539900	0.62803000	-1.04490000
H	-5.57561700	1.01187800	-0.25525300
C	2.45846500	-2.58059000	-0.71105100
H	1.64468900	-1.85051800	-0.70008000
Cl	-0.01339500	0.35485800	-0.12107100
C	2.07958800	-3.65050100	-1.72395900
C	0.84237600	-3.59190000	-2.37378600
C	2.94869000	-4.70743700	-2.02550700

C	0.47738600	-4.56614700	-3.30465500
H	0.16015000	-2.77668800	-2.15155500
C	2.58385300	-5.68697200	-2.94945300
H	3.91988300	-4.77234500	-1.54336500
C	1.34682500	-5.61828900	-3.59330000
H	-0.48590100	-4.50274900	-3.80076100
H	3.26799500	-6.50044300	-3.16904700
H	1.06450800	-6.37828200	-4.31472800
C	1.94887000	6.01159000	-0.25788900
C	2.59677200	7.19770200	0.10163200
C	0.92182700	6.06814200	-1.20648700
C	2.23279900	8.41513500	-0.47600800
H	3.38671500	7.17064600	0.84722200
C	0.55230200	7.28325000	-1.78468200
H	0.39787600	5.16096000	-1.49234000
C	1.20811000	8.46154300	-1.42246700
H	2.74325300	9.32620700	-0.17955700
H	-0.24929300	7.30933800	-2.51642700
H	0.91900100	9.40736000	-1.86954600
C	-5.73072000	-0.37125900	-1.86968200
C	-7.12666900	-0.28710400	-1.88311900
C	-5.10870900	-1.34237300	-2.66194900
C	-7.88790500	-1.14997200	-2.67307100
H	-7.62353900	0.45318900	-1.26204500
C	-5.86557000	-2.20982400	-3.45066300
H	-4.02646800	-1.43151800	-2.65932000
C	-7.25864500	-2.11545400	-3.46035400
H	-8.97075700	-1.07350400	-2.66525500
H	-5.36686100	-2.96047000	-4.05606300
H	-7.84792000	-2.79194500	-4.07119700
C	3.76698700	-1.85380900	-1.06594800
H	3.99537800	-1.08344000	-0.32363300
H	4.60888400	-2.55106300	-1.10306800
H	3.67239400	-1.37274200	-2.04418300
C	-4.43740500	1.80306500	-1.90566600
H	-3.92668600	2.54857300	-1.28795300
H	-3.74850000	1.46148200	-2.68682300
H	-5.28770600	2.28132500	-2.39808500
C	3.38609100	3.95609700	-0.59099000
H	3.76643700	3.04599800	-0.11647600
H	2.89942000	3.68382000	-1.53459100
H	4.23216700	4.60570600	-0.82880100
H	-0.43048500	0.17319500	2.21412000

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Charge: 0 Multiplicity: 1

N	0.12903300	0.21296200	2.65548300
C	1.44926800	0.34435900	3.39092300
H	1.25904100	0.03071000	4.42006400
H	1.72765400	1.39807200	3.39632100
C	-0.76634800	1.40839600	2.93246600
H	-0.67348000	1.61326600	4.00158100
H	-1.79404300	1.10829900	2.72578900
C	-0.57610900	-1.07710900	3.03472300
H	-1.15710000	-0.85485300	3.93197000
H	0.17982600	-1.81610300	3.29531300
C	2.58308400	-0.47361000	2.76655400
H	2.27801700	-1.50905100	2.58905600
H	3.40191600	-0.48983300	3.48764700
C	-0.42667500	2.65023200	2.10476000
H	0.64475200	2.86861100	2.12905500

H	-0.94450700	3.49305000	2.56543800
C	-1.47238600	-1.64000200	1.92672300
H	-2.01560500	-0.84439200	1.40898400
H	-2.20918700	-2.28867300	2.40279100
N	3.06988000	0.07376700	1.51777800
H	2.50580800	-0.12664200	0.69109600
N	-0.84387700	2.55389000	0.72251400
H	-0.25409900	1.98508200	0.11356700
N	-0.75318700	-2.40715100	0.92547100
H	-0.42573600	-1.88426700	0.11659600
C	3.97691400	1.08399700	1.41756600
C	-2.07786600	2.89231000	0.26072600
C	-0.36067400	-3.68779700	1.10070800
S	4.81832100	1.69904800	2.75792500
S	-3.25273000	3.63917200	1.23309600
S	-0.66399800	-4.56166800	2.53479300
N	4.15966500	1.53313200	0.15567300
H	3.57976800	1.12416300	-0.56828300
N	-2.27438700	2.59891800	-1.04478500
H	-1.51868800	2.13177700	-1.53239500
N	0.30670400	-4.27922900	0.08446700
H	0.56649600	-5.23655000	0.27511800
C	5.06309400	2.60806600	-0.25623300
H	5.90815800	2.58392800	0.43448400
C	-3.48915800	2.86081100	-1.81608600
H	-3.93366200	3.76695900	-1.39926700
C	0.49635600	-3.78463200	-1.28374500
H	0.84035000	-2.74572300	-1.23254000
C	4.42452300	3.99103400	-0.16988500
C	5.15539500	5.05934300	0.35918700
C	3.13452100	4.23551400	-0.65571400
C	4.61459200	6.34586800	0.40059600
H	6.15307000	4.88199300	0.75094600
C	2.58787900	5.51862000	-0.61227200
H	2.54486000	3.42101200	-1.06636900
C	3.32752500	6.57954300	-0.08529400
H	5.19573300	7.16134600	0.81981900
H	1.58474000	5.68968600	-0.99046100
H	2.90196400	7.57734900	-0.04992700
C	-4.52102200	1.74164600	-1.71434900
C	-4.15009500	0.39293700	-1.74773600
C	-5.88048400	2.06257800	-1.64334000
C	-5.11660300	-0.61319500	-1.70934600
H	-3.10047200	0.11947100	-1.79834300
C	-6.85117100	1.06017800	-1.60778500
H	-6.18213800	3.10572800	-1.60473100
C	-6.47144200	-0.28260200	-1.64012500
H	-4.80939100	-1.65399000	-1.73540300
H	-7.90121900	1.32873700	-1.54591700
H	-7.22346200	-1.06459100	-1.60740400
C	-0.77897500	-3.82497400	-2.12342300
C	-0.97091500	-2.86393300	-3.12278900
C	-1.73649200	-4.83223900	-1.96321200
C	-2.09222300	-2.91177200	-3.95213400
H	-0.24119300	-2.06876600	-3.24791700
C	-2.86044500	-4.88096800	-2.78953900
H	-1.61259000	-5.57847600	-1.18479100
C	-3.04106000	-3.92254200	-3.78832100
H	-2.22720800	-2.15680900	-4.72028800
H	-3.59530800	-5.66779000	-2.65053000
H	-3.91568900	-3.95997000	-4.42980800

C	5.56874600	2.30704300	-1.67504600
H	6.08720800	1.34351800	-1.70222400
H	4.74134300	2.28165100	-2.39357800
H	6.26318800	3.08776900	-1.99587100
C	-3.09211900	3.12467400	-3.27673700
H	-2.40871500	3.97714000	-3.34257300
H	-2.60487000	2.24718300	-3.71751200
H	-3.98278800	3.34342100	-3.87118500
C	1.61853200	-4.61036400	-1.93137100
H	2.54353100	-4.52408800	-1.35278100
H	1.33608600	-5.66736500	-1.99369900
H	1.80591800	-4.25293600	-2.94647100
Cl	0.70361500	0.08406700	-0.68711500
H	0.32519700	0.18476100	1.63340200

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Charge: -1 Multiplicity: 1

C	0.56378400	-1.27001100	-2.59360200
N	-0.04951000	0.09541400	-2.34114500
C	-1.43815700	0.18770900	-2.93717700
H	-1.31004600	0.45319300	-3.99002500
C	-2.34990300	1.19295700	-2.22389200
N	-2.81317100	0.74142000	-0.93170500
C	-3.83985200	-0.12723100	-0.73675900
N	-4.01922500	-0.47666800	0.55508800
H	-3.33943800	-0.10258200	1.22126200
C	-5.06707200	-1.35491000	1.06042100
C	-6.37297200	-0.62230700	1.36071700
C	-6.38632200	0.67394900	1.88934000
C	-7.59294200	1.30104200	2.20877800
C	-8.80621300	0.63878400	2.00510100
C	-8.80302300	-0.65432500	1.47613500
C	-7.59410800	-1.27614100	1.15626400
H	-7.59948000	-2.27762800	0.73269500
H	-9.74035800	-1.17568600	1.30340300
H	-9.74456700	1.12786000	2.24995000
H	-7.58382300	2.30865900	2.61473300
H	-5.45024700	1.20245200	2.04412100
C	-4.54150700	-2.08253500	2.30892800
H	-5.30557100	-2.76456100	2.69250200
H	-4.29440500	-1.37068700	3.10455900
H	-3.64355100	-2.66022400	2.06818000
H	-5.27190000	-2.09343100	0.28019900
S	-4.79576100	-0.71844600	-2.01470900
H	-2.29672400	1.02859800	-0.09587600
H	-1.84906700	2.15554300	-2.08370500
H	-3.20841700	1.35988600	-2.87977800
H	-1.89825300	-0.79840100	-2.88633500
C	0.83480300	1.19101200	-2.90566100
H	1.12672300	0.86140700	-3.90706500
C	2.07313900	1.52345000	-2.06467200
N	1.77897400	2.23431000	-0.84192500
C	1.74347800	3.58764800	-0.70816800
N	1.25274100	4.00324100	0.47660600
C	1.22540600	5.38435300	0.94992800
C	2.46339800	5.74472300	1.76762800
C	3.12933400	6.95259300	1.53033000

C	4.23781900	7.32341500	2.29663200
C	4.69783000	6.48318000	3.31251500
C	4.04203500	5.27243900	3.55458000
C	2.93356800	4.90712000	2.78871400
H	2.43722600	3.96094700	2.98575600
H	4.39390500	4.60985900	4.34022300
H	5.56179500	6.76531300	3.90724300
H	4.74469200	8.26258800	2.09336000
H	2.78288000	7.60521700	0.73295800
C	-0.06596400	5.61679500	1.75074000
H	-0.10435000	6.65073800	2.10667200
H	-0.94313500	5.42779100	1.12339100
H	-0.11628500	4.95482700	2.62179400
H	1.21321500	6.02030200	0.06212100
H	0.94033000	3.27863700	1.13530200
S	2.27099500	4.64331800	-1.93937900
H	1.34072200	1.67007600	-0.11096200
H	2.71581100	2.15202500	-2.68471700
H	2.63826400	0.62006500	-1.81418900
H	0.22058800	2.08714300	-3.00463800
H	0.39597300	-1.48364700	-3.65298800
C	0.00288100	-2.40556800	-1.73400500
N	0.40113600	-2.31913700	-0.34821900
C	1.04289500	-3.27899700	0.36474600
N	1.25550300	-2.93723900	1.65349000
C	1.89628600	-3.76959900	2.66735600
C	0.88699900	-4.52254700	3.53009700
C	1.09510700	-5.87442900	3.82643800
C	0.21077500	-6.57145800	4.65448200
C	-0.89936900	-5.92035200	5.19617200
C	-1.11722000	-4.57082400	4.90281100
C	-0.23075600	-3.87671200	4.07720300
H	-0.41492200	-2.82943900	3.85359800
H	-1.97895700	-4.05574600	5.31781600
H	-1.59145200	-6.45920400	5.83688400
H	0.38594900	-7.62211400	4.86843700
H	1.95212700	-6.38877900	3.39888400
C	2.82125400	-2.89145600	3.52673500
H	3.58688000	-2.41942500	2.90229600
H	2.25394100	-2.10349400	4.03372700
H	3.31544700	-3.49977200	4.29048100
H	2.49825700	-4.50623800	2.13148800
H	0.84648600	-2.05494500	1.98064300
S	1.54379100	-4.76067900	-0.31577900
H	0.20148200	-1.43089000	0.12369700
H	0.39746000	-3.34005400	-2.14061000
H	-1.09041900	-2.45664100	-1.81598100
H	1.63702900	-1.18123300	-2.42218600
H	-0.12510300	0.23961600	-1.30312800
S	-0.36756300	0.68687400	1.80344700
O	0.06585400	0.35209000	0.38087700
O	0.44079900	1.83813800	2.25545100
O	-0.13352800	-0.50821000	2.63711600
O	-1.81087900	1.03961200	1.76108800

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Charge: -1 Multiplicity: 1

C	0.51208500	-1.53352900	2.34525500
N	-0.06184900	-0.13713800	2.19181700
C	-1.41857100	-0.02783500	2.85486300
H	-1.23385500	0.15245900	3.91734800

C	-2.31362000	1.06821500	2.26286000
N	-2.84516200	0.74441600	0.95818400
C	-3.91837900	-0.05821100	0.73190800
N	-4.17892600	-0.26145200	-0.57708400
H	-3.51205000	0.14885500	-1.23666500
C	-5.21692100	-1.13572100	-1.11227600
C	-4.76728600	-2.59025600	-1.23174500
C	-3.49574400	-2.92596500	-1.71516400
C	-3.12056200	-4.26355000	-1.85722000
C	-4.01327600	-5.28564500	-1.52343300
C	-5.28354400	-4.95992900	-1.04241800
C	-5.65354000	-3.62053100	-0.89661300
H	-6.63792300	-3.37246700	-0.50708800
H	-5.98262800	-5.74598800	-0.77079100
H	-3.71825300	-6.32538300	-1.63101700
H	-2.12824000	-4.50536800	-2.22622700
H	-2.78679700	-2.14497800	-1.97646700
C	-5.67753700	-0.58066500	-2.46979900
H	-6.47291000	-1.20922000	-2.88072500
H	-6.05774200	0.44006700	-2.35758800
H	-4.85209200	-0.56801100	-3.19022900
H	-6.05479700	-1.10156300	-0.41180900
S	-4.84667900	-0.72240000	1.99446900
H	-2.33969000	1.06857000	0.13114600
H	-1.78069400	2.02002500	2.18186100
H	-3.13849000	1.21274900	2.96525100
H	-1.92581000	-0.98653700	2.75288200
C	0.88751200	0.89471100	2.77014000
H	1.21958200	0.49870500	3.73418300
C	2.09037000	1.23711100	1.88280800
N	1.75298600	2.00994800	0.70867400
C	1.64259200	3.36668600	0.67090200
N	1.16158700	3.83949800	-0.49568300
C	0.91353000	5.24332600	-0.81102500
C	-0.51004600	5.68236800	-0.47557200
C	-1.61839000	4.89226600	-0.81071800
C	-2.91398800	5.33470800	-0.53499600
C	-3.12215100	6.57486500	0.07554000
C	-2.02349300	7.36903600	0.41111700
C	-0.72812300	6.92192000	0.13711700
H	0.12394700	7.53870900	0.41207900
H	-2.17189700	8.33139500	0.89302100
H	-4.13066600	6.91589900	0.29101300
H	-3.76106700	4.70821800	-0.79941900
H	-1.47771200	3.92385400	-1.28289900
C	1.23747600	5.48330200	-2.29497800
H	1.06671400	6.53323700	-2.55094900
H	0.60129600	4.86804100	-2.94042000
H	2.28396400	5.23618500	-2.50197300
H	1.59938100	5.83143100	-0.19729300
H	0.88289100	3.14774700	-1.20320600
S	2.10052300	4.35628800	1.98082700
H	1.30057800	1.48131300	-0.03860800
H	2.77914500	1.81810800	2.49951800
H	2.61866100	0.33528500	1.55912000
H	0.31332900	1.80399000	2.95186600
H	0.39662800	-1.79379300	3.40140300
C	-0.13611500	-2.60627800	1.46280200
N	0.16932400	-2.46589900	0.05824900
C	1.01426400	-3.24924400	-0.66023800
N	1.11569900	-2.87839900	-1.95513600

C	2.04289800	-3.44045300	-2.93253000
C	3.36057400	-2.67184300	-2.99758600
C	4.57121700	-3.36896700	-3.08397700
C	5.78579700	-2.68603600	-3.19205200
C	5.80310300	-1.28975600	-3.21221100
C	4.59920600	-0.58472600	-3.12359100
C	3.38756800	-1.27048700	-3.01873700
H	2.46046500	-0.70821300	-2.94869900
H	4.60095100	0.50138700	-3.13655600
H	6.74526800	-0.75504800	-3.29130100
H	6.71569600	-3.24471700	-3.25185900
H	4.56494000	-4.45587200	-3.05747700
C	1.35553700	-3.48903500	-4.30683300
H	0.45090200	-4.10410800	-4.25995800
H	2.03378600	-3.91805300	-5.05055400
H	1.07597600	-2.48450000	-4.64192600
H	2.26171100	-4.45938300	-2.60622500
H	0.56396000	-2.06838300	-2.25922000
S	1.83923300	-4.58336000	0.00750900
H	-0.10896800	-1.57837300	-0.36994400
H	0.25308200	-3.56988800	1.79963400
H	-1.22323100	-2.62677800	1.59974400
H	1.57665300	-1.47415900	2.11671500
H	-0.17873000	0.06308000	1.16753600
S	-0.55924800	0.67629000	-1.90775400
O	-0.10673900	0.24688600	-0.51984600
O	0.34840100	1.75204800	-2.36099100
O	-0.49085500	-0.50630300	-2.78935400
O	-1.95342900	1.17953100	-1.79010500

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Charge: -1 Multiplicity: 1

C	0.74555600	-1.47125800	-1.83729000
N	0.15433900	-0.08175000	-1.71976500
C	-1.08625100	0.03271700	-2.57584600
H	-0.74151400	0.17487900	-3.60449200
C	-2.03733300	1.16077800	-2.16086100
N	-2.77885900	0.88196800	-0.95402200
C	-3.89802700	0.11768000	-0.88990400
N	-4.32233300	-0.11594600	0.37216100
H	-3.72462700	0.24276400	1.11883700
C	-5.52017000	-0.85607200	0.74746700
C	-6.77510300	0.01272800	0.79498100
C	-6.74386100	1.32473400	1.28300800
C	-7.91507400	2.08060900	1.37072700
C	-9.13752400	1.53367900	0.97194200
C	-9.17828300	0.22624700	0.48142500
C	-8.00385400	-0.52473400	0.39349900
H	-8.04019500	-1.53736000	-0.00105500
H	-10.12107600	-0.20637300	0.15856000
H	-10.04772800	2.12274000	1.03676000
H	-7.87102900	3.09803400	1.74897800
H	-5.79858100	1.76370800	1.58867200
C	-5.27093400	-1.54171300	2.10097500
H	-6.15164300	-2.11908300	2.39616100
H	-5.07285300	-0.80289800	2.88579900
H	-4.41196400	-2.21715800	2.03665400
H	-5.67609400	-1.62309900	-0.01603300
S	-4.68545700	-0.48756900	-2.27340600
H	-2.37816600	1.17043800	-0.05221300
H	-1.49927800	2.10241300	-2.01554000

H	-2.73559300	1.30487100	-2.98939200
H	-1.62265200	-0.91469600	-2.52400300
C	1.17628500	0.95329700	-2.13438000
H	1.68915300	0.54844400	-3.01173400
C	2.18279700	1.32787200	-1.04011800
N	1.64270000	2.20881400	-0.03100600
C	1.51746000	3.55469400	-0.15840700
N	0.84980800	4.13604400	0.86152200
C	0.64689700	5.56806500	1.04130500
C	1.79122500	6.24297800	1.79447300
C	2.21840100	7.51920400	1.40968900
C	3.22579000	8.18163400	2.11542300
C	3.82396100	7.57046500	3.21981200
C	3.40693900	6.29475300	3.60968700
C	2.39804700	5.63766000	2.90221900
H	2.08746800	4.64379400	3.21159100
H	3.86781800	5.80887600	4.46507000
H	4.61094500	8.08010200	3.76806800
H	3.54811600	9.16903300	1.79697300
H	1.76548800	7.99490500	0.54320700
C	-0.69586500	5.79306300	1.75552200
H	-0.87539200	6.86415200	1.88591700
H	-1.51760800	5.36667600	1.17138300
H	-0.69746300	5.32725100	2.74728700
H	0.59783600	6.01258500	0.04365800
H	0.46430100	3.49888700	1.56422700
S	2.13890900	4.41383500	-1.49198500
H	1.22713900	1.78827000	0.80366200
H	3.02071300	1.82295500	-1.53726200
H	2.57436700	0.44059400	-0.53472000
H	0.64189200	1.85262700	-2.44064300
H	0.73696200	-1.70913600	-2.90438200
C	0.01514000	-2.56194200	-1.04592000
N	0.48098500	-2.67567100	0.32409900
C	0.86406600	-3.83293900	0.89747000
N	1.23068600	-3.78659200	2.20038400
C	1.51165900	-2.60205100	3.01991500
C	2.83589400	-1.92912400	2.65821300
C	2.96552200	-0.54140500	2.80434800
C	4.18145200	0.09166000	2.53537800
C	5.28604000	-0.65377600	2.11525400
C	5.16356500	-2.03714300	1.96286800
C	3.94685200	-2.66864800	2.23289300
H	3.86317900	-3.74320100	2.09877400
H	6.01352400	-2.62684300	1.63093600
H	6.23031300	-0.16092600	1.90264200
H	4.26073500	1.16922100	2.64623000
H	2.10743500	0.05090800	3.10996300
C	1.49374700	-3.03490500	4.49447700
H	0.51820700	-3.45625000	4.75709400
H	2.27047600	-3.78386400	4.69213600
H	1.68445800	-2.17234400	5.13758900
H	0.70165000	-1.87708700	2.89074100
H	1.51843100	-4.68255600	2.56630000
S	0.91186100	-5.33572800	0.08341700
H	0.31918000	-1.83902400	0.89349300
H	0.20926600	-3.51761500	-1.53563700
H	-1.06984200	-2.40605600	-1.06182400
H	1.78399500	-1.41851300	-1.50766400
H	-0.10176800	0.07023500	-0.69884300
S	-0.80050600	0.70907100	2.12661500

O	-0.26483400	-0.05997100	0.93046200
O	0.18336800	1.78440800	2.43589400
O	-0.95453800	-0.21265200	3.25524600
O	-2.10363900	1.31735900	1.73325500

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Charge: -1 Multiplicity: 1

C	0.56731500	-1.58303800	1.98468000
N	-0.08548000	-0.23132500	1.79851500
C	-1.37498000	-0.15075300	2.58531400
H	-1.09382500	0.07114900	3.61866800
C	-2.37169500	0.88765300	2.05715700
N	-3.06494800	0.46850000	0.86112000
C	-4.14370600	-0.35798600	0.83595800
N	-4.55092800	-0.67697100	-0.41104200
H	-3.96186700	-0.32836200	-1.17340100
C	-5.64574600	-1.57766900	-0.74994100
C	-5.22651900	-3.04593300	-0.79550500
C	-3.99255100	-3.44277800	-1.32748800
C	-3.65782000	-4.79715800	-1.40425400
C	-4.55073300	-5.77344800	-0.95444900
C	-5.78260900	-5.38526400	-0.42217400
C	-6.11350400	-4.03040300	-0.34370200
H	-7.06823600	-3.73344900	0.08383400
H	-6.48158400	-6.13391200	-0.05967600
H	-4.28621200	-6.82536300	-1.01255600
H	-2.69541600	-5.08775600	-1.81583400
H	-3.28001900	-2.69927200	-1.67520600
C	-6.24793800	-1.13291000	-2.09339600
H	-7.08608900	-1.78217500	-2.36249100
H	-6.60835000	-0.10092400	-2.02893200
H	-5.50377300	-1.19265600	-2.89556700
H	-6.40360900	-1.47044400	0.03034500
S	-4.90758400	-0.91559700	2.25257800
H	-2.67027200	0.72602600	-0.04781700
H	-1.87872900	1.84071800	1.84455300
H	-3.09905900	1.06289500	2.85367000
H	-1.84905200	-1.13146500	2.56716600
C	0.86128000	0.86259400	2.25006500
H	1.33772500	0.49367400	3.16228900
C	1.91813700	1.26888100	1.21389100
N	1.44619100	2.24235100	0.24595500
C	1.37896000	3.56584900	0.49138900
N	0.84680500	4.35099500	-0.47637800
C	0.60415400	4.01105100	-1.88476000
C	1.88258400	3.99019100	-2.72199800
C	2.90298200	4.93049600	-2.53014000
C	4.03103200	4.93429700	-3.35357900
C	4.15192800	3.99679500	-4.38279000
C	3.14088000	3.05231800	-4.57569000
C	2.01419800	3.04673500	-3.74912900
H	1.23724600	2.29893600	-3.88380300
H	3.23050200	2.31154800	-5.36510600
H	5.02931500	3.99857300	-5.02317600
H	4.81525500	5.66783000	-3.18889000
H	2.82735900	5.66034200	-1.72909800
C	-0.41269200	5.01736800	-2.44558800
H	-0.62907200	4.78391800	-3.49094000
H	-0.01523000	6.03865900	-2.40209800
H	-1.34706800	4.97595100	-1.87700300
H	0.14356000	3.02093800	-1.93801800

H	0.83831400	5.33138800	-0.23373200
S	1.91292700	4.28171700	1.94644800
H	0.88545500	1.83372200	-0.50592200
H	2.76002500	1.69995600	1.75768900
H	2.28688000	0.40237300	0.65842500
H	0.26672000	1.73737800	2.51263200
H	0.55398700	-1.78251000	3.06048500
C	-0.09670200	-2.73210000	1.21747600
N	0.17611300	-2.72591300	-0.19909600
C	1.27054700	-3.27257900	-0.78273700
N	1.33108100	-3.06682800	-2.11828100
C	2.38187300	-3.54442400	-3.00833100
C	3.60875000	-2.63564900	-3.04491200
C	4.88178700	-3.20131800	-3.18509800
C	6.01894700	-2.39532500	-3.27413300
C	5.89588600	-1.00462700	-3.22073400
C	4.62979700	-0.43087700	-3.07889800
C	3.49515400	-1.24131800	-2.99326800
H	2.51837600	-0.78129400	-2.87751600
H	4.52082800	0.64869900	-3.03475200
H	6.77805700	-0.37397000	-3.28282600
H	6.99901000	-2.85330100	-3.37482700
H	4.98540100	-4.28351800	-3.21222200
C	1.78581200	-3.72567600	-4.41424400
H	0.95096300	-4.43385700	-4.38919700
H	2.54913100	-4.10680600	-5.09849000
H	1.42260000	-2.77153800	-4.81239700
H	2.70308100	-4.51950100	-2.63196400
H	0.59017800	-2.48790700	-2.51608200
S	2.44433100	-4.15137800	0.08320100
H	-0.44880700	-2.19313800	-0.81806000
H	0.28537800	-3.65921200	1.65185400
H	-1.18199600	-2.73095600	1.35377000
H	1.60647300	-1.49816700	1.66436400
H	-0.28819300	-0.08438600	0.76697600
S	-1.09825300	0.11294100	-2.11160300
O	-0.34228700	0.42058300	-0.83288200
O	-0.41805800	0.75303600	-3.24114900
O	-1.14065800	-1.37110500	-2.27162200
O	-2.48473100	0.63600800	-1.94876500