Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPLEMENTARY MATERIAL

to

Sándor Góbi,[a] Elemér Vass,[b] Gábor Magyarfalvi,[a] György Tarczay[a,*]

[a]Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös University, PO Box 32, H-1518, Budapest 112, Hungary

[b]Laboratory for Chiroptical Structure Analysis, Institute of Chemistry, Eötvös University, PO Box 32, H-1518, Budapest 112, Hungary

e-mail: tarczay@chem.elte.hu

Effects of strong and weak hydrogen bond formation on VCD spectra: A case study of 2-chloropropionic acid

Cartesian coordinates (in Å) of S-(–)-2-chloropropionic acid monomers at the B3LYP / aug-cc-pVTZ level of theory

conformer	atomic label	x	y	z
1	C	0.868877	1.205364	0.048846
	H	0.832921	1.451824	-1.009536
	H	0.190501	1.876355	0.578979
	H	1.878371	1.362628	0.422811
	C	0.443753	-0.226293	0.281329
	H	0.481227	-0.504010	1.330386
	C	-0.941088	-0.531961	-0.269729
	O	-1.483602	0.081242	-1.148813
	O	-1.502154	-1.583039	0.362679
	H	-2.361220	-1.748579	-0.053592
	Cl	1.592413	-1.383532	-0.543358

conformer	atomic label	x	y	z
2	C	-0.755265	1.146431	0.007784
	H	-0.740043	1.178562	1.094543
	H	-0.010286	1.847352	-0.374665
	H	-1.736068	1.460596	-0.343520
	C	-0.445692	-0.249430	-0.501187
	H	-0.498754	-0.305755	-1.582640
	C	0.932613	-0.752905	-0.107251
	O	1.758301	-1.123552	-0.899371
	O	1.144857	-0.708192	1.222213
	H	2.036094	-1.050711	1.384655
	Cl	-1.685756	-1.442394	0.099439

conformer	atomic label	x	y	z
3	C	-0.383100	1.273468	0.352980
	H	-0.436396	1.046536	1.416799
	H	0.507568	1.871755	0.165531
	H	-1.263533	1.847147	0.072216
	C	-0.295521	0.000123	-0.473403
	H	-0.297263	0.225639	-1.535954
	C	1.000842	-0.767991	-0.183844
	O	2.053548	-0.256342	-0.447334
	O	0.919479	-1.981848	0.372044
	H	-0.012832	-2.232801	0.475980
	Cl	-1.792792	-1.025686	-0.215016

Relative energies and populations at 273 K of S-(–)-2-chloropropionic acid monomers at the B3LYP / aug-cc-pVTZ level of theory

conformer	ΔG^o_{0K} / kJ mol^{-1}	ΔG^o_{273K} / kJ mo^{-1}	N_i / N
1	0.0	0.0	0.589
2	1.7	1.3	0.346
3	5.5	5.4	0.065

Potential energy and rotary strengths (in 10^{-44} esu^2 cm^2) scan of cis-S-(–)-2-chloropropionic acid (see Fig. 2.)

ψ / °	ΔE / kJ mol^{-1}	R_{v6}	R_{v7}	R_{v8}	R_{v9}	R_{v10}	R_{v11}	R_{v12}
–200	4.4	–68	–1	–5	2	1	18	–48
–180	4.4	–47	–2	–8	3	5	22	–39
–160	5.8	–10	–1	–9	3	12	13	–16
–140	3.8	18	1	–8	1	4	9	–3
–120	1.3	23	5	–5	–1	–15	14	–3
–100	0.0	9	2	4	–2	–34	20	–13
–80	1.0	–11	2	6	–1	–46	24	–31
–60	3.1	–28	5	3	1	–42	19	–48
–40	4.1	–33	5	–1	1	–29	4	–46
–20	4.7	–23	2	–4	2	–27	–2	–33
0	6.3	–1	1	–7	3	–34	3	–12
20	8.7	29	0	–10	3	–38	12	12
40	10.1	59	1	–8	3	–33	23	22
60	8.5	70	3	–4	3	–20	31	–1
80	4.7	51	3	2	3	7	20	–30
100	2.1	11	2	4	3	23	7	–42
120	1.8	–31	1	2	2	17	7	–46
140	2.8	–61	0	–2	2	6	11	–47
160	4.4	–68	–1	–5	2	1	18	–48
180	4.4	–47	–2	–8	3	5	22	–39
200	5.8	–10	–1	–9	3	12	13	–16

Cartesian coordinates (in Å) of S-(–)-2-chloropropionic acid dimers at the B3LYP / aug-cc-pVTZ level of theory

1-1	C	-4.133899	-0.493304	-0.918752
	H	-3.829002	-0.073262	-1.874126
	H	-3.883961	-1.556253	-0.914429
	H	-5.211025	-0.389762	-0.806259
	C	-3.422907	0.196409	0.223638
	H	-3.718270	-0.193761	1.192477
	C	-1.906557	0.145839	0.113157
	O	-1.332481	0.112332	-0.964738
	O	-1.307307	0.135879	1.282442
	H	-0.311849	0.132810	1.170539
	Cl	-3.861749	1.968066	0.282329
	C	4.134102	-0.485014	0.921534
	H	3.828075	-0.060852	1.874704
	H	3.885647	-1.548317	0.922119
	H	5.211162	-0.380548	0.809252
	C	3.422901	0.198405	-0.224548
	H	3.719311	-0.195906	-1.191369
	C	1.906603	0.146436	-0.114626
	O	1.331846	0.116819	0.962986
	O	1.307585	0.129534	-1.284006
	H	0.312445	0.124136	-1.171137
	Cl	3.859329	1.970313	-0.291187

1-2	C	3.862962	1.604405	-0.419142
	H	3.548835	1.456132	-1.449378
	H	3.434557	2.542335	-0.060051
	H	4.947506	1.680779	-0.379771
	C	3.389287	0.466643	0.456617
	H	3.700177	0.580680	1.490089
	C	1.883457	0.256029	0.414581
	O	1.219209	0.502734	-0.580824
	O	1.397678	-0.202745	1.545329
	H	0.409739	-0.355407	1.470646
	Cl	4.130135	-1.114334	-0.080267
	C	-3.863912	-1.381668	-0.901229
	H	-3.632016	-0.852912	-1.822402
	H	-3.375392	-2.358107	-0.926569
	H	-4.939251	-1.535937	-0.838169
	C	-3.380828	-0.605329	0.307962
	H	-3.637418	-1.098284	1.239058
	C	-1.881293	-0.359959	0.329473
	O	-1.219883	-0.597119	1.330891
	O	-1.392845	0.095067	-0.799679
	H	-0.406327	0.252303	-0.722824
	Cl	-4.194377	1.024694	0.395660

2-2	C	4.161803	-0.696286	0.362233
	H	4.007147	-0.521345	1.424003
	H	3.822617	-1.706129	0.121483
	H	5.224741	-0.627830	0.139679
	C	3.392810	0.308946	-0.472254
	H	3.565034	0.175056	-1.534427
	C	1.889171	0.277064	-0.255018
	O	1.117809	0.247029	-1.204468
	O	1.525096	0.265736	1.004661
	H	0.525600	0.262522	1.086553
	Cl	3.951350	2.006920	-0.112511
	C	-4.161695	-0.695431	-0.360645
	H	-4.006924	-0.522977	-1.422796
	H	-3.822379	-1.704651	-0.117501
	H	-5.224698	-0.626670	-0.138418
	C	-3.392895	0.311836	0.471538
	H	-3.565155	0.180337	1.534007
	C	-1.889236	0.279572	0.254263
	O	-1.117762	0.250844	1.203672
	O	-1.525104	0.265486	-1.005369
	H	-0.525625	0.261109	-1.086635
	Cl	-3.951704	2.008861	0.107951

Cartesian coordinates (in Å) of S-(–)-2-chloropropionic acid – $CHCl_3$ complexes at the B3LYP/aug-cc-pVTZ level of theory.

1a	C	-1.246174	-1.403036	0.812800
	H	-0.471216	-1.722320	0.120473
	H	-0.769089	-1.097558	1.745804
	H	-1.909538	-2.240156	1.019512
	C	-2.034451	-0.244713	0.245875
	H	-2.827263	0.081032	0.912129
	C	-1.166729	0.949558	-0.119011
	O	0.002068	0.893092	-0.404016
	O	-1.862960	2.098270	-0.080922
	H	-1.270972	2.814720	-0.355871
	Cl	-2.890391	-0.732395	-1.291389
	C	3.178479	0.144630	-0.529729
	H	2.122605	0.362140	-0.593743
	Cl	3.380430	-1.625568	-0.634039
	Cl	3.767810	0.760922	1.037692
	Cl	3.997391	0.961382	-1.885566

1b	C	-2.425177	1.298847	0.467302
	H	-1.983188	1.332228	1.460070
	H	-2.029169	2.134499	-0.112840
	H	-3.504093	1.411743	0.548326
	C	-2.088689	-0.000742	-0.227278
	H	-2.527527	-0.067027	-1.218005
	C	-0.592572	-0.257493	-0.323988
	O	0.224728	0.192133	0.442043
	O	-0.289561	-1.037657	-1.368798
	H	0.671041	-1.201219	-1.368924
	Cl	-2.786426	-1.421307	0.684499
	C	3.370634	-0.430345	0.252025
	H	2.394286	-0.081719	0.560695
	Cl	4.090592	-1.373331	1.571590
	Cl	4.372223	0.973964	-0.170675
	Cl	3.102897	-1.472574	-1.196043

2a	C	2.051603	-0.037996	1.405867
	H	2.977359	0.454389	1.118149
	H	1.443027	0.664045	1.979661
	H	2.284223	-0.890155	2.041226
	C	1.277110	-0.502285	0.186562
	H	0.372367	-1.033093	0.461439
	C	0.861354	0.624250	-0.741943
	O	-0.276418	0.817818	-1.093803
	O	1.886089	1.406160	-1.113498
	H	1.537540	2.086520	-1.708692
	Cl	2.254387	-1.693199	-0.785782
	C	-3.239328	-0.331922	-0.392787
	H	-2.309144	0.086552	-0.749812
	Cl	-4.123991	-1.006397	-1.782206
	Cl	-4.169567	0.970381	0.391396
	Cl	-2.826610	-1.615069	0.784223

2b	C	2.687752	-1.104426	-0.001322
	H	2.697103	-1.120856	1.085755
	H	2.179954	-2.001874	-0.361036
	H	3.712680	-1.119168	-0.366485
	C	1.971043	0.127065	-0.522213
	H	1.991424	0.180440	-1.604981
	C	0.512185	0.215362	-0.106641
	O	-0.388299	0.370930	-0.897404
	O	0.332748	0.075127	1.210738
	H	-0.618354	0.153198	1.406121
	Cl	2.804424	1.645815	0.044383
	C	-3.487680	0.519579	-0.053119
	H	-2.556730	0.528685	-0.604062
	Cl	-4.337815	2.052260	-0.330368
	Cl	-3.045794	0.348826	1.687837
	Cl	-4.454643	-0.870963	-0.587201

Coordinates (in Å) of S-(–)-2-chloropropionic acid – $CHCl_3$ complexes at the MP2/6-31++G level of theory.**

1a	C	1.753167	1.718242	-0.053779
	H	1.787537	1.852601	-1.132609
	H	0.717917	1.789905	0.278335
	H	2.327091	2.509058	0.425068
	C	2.321740	0.371299	0.335212
	H	2.284867	0.212106	1.412163
	C	1.595854	-0.777156	-0.336589
	O	0.829614	-0.659538	-1.283013
	O	1.890684	-1.958858	0.243491
	H	1.401219	-2.645722	-0.242498
	Cl	4.052874	0.251445	-0.126793
	C	-1.980831	0.036808	-0.151970
	H	-1.216508	-0.090049	-0.909218
	Cl	-2.452250	1.738765	-0.125097
	Cl	-1.266582	-0.448836	1.397029
	Cl	-3.346048	-0.998779	-0.572921

1b	C	3.233180	1.828739	-0.248636
	H	2.915870	1.856100	-1.288324
	H	2.629438	2.536286	0.320991
	H	4.278292	2.123365	-0.179432
	C	3.049789	0.439400	0.322358
	H	3.354885	0.381997	1.365104
	C	1.614740	-0.033744	0.209746
	O	0.838315	0.322444	-0.665843
	O	1.302143	-0.902196	1.192792
	H	0.384103	-1.200547	1.044247
	Cl	4.057614	-0.757591	-0.558411
	C	-2.187143	0.067144	-0.241449
	H	-1.338127	0.257193	-0.885515
	Cl	-3.664453	0.151480	-1.196074
	Cl	-2.170563	1.281862	1.038308
	Cl	-1.964452	-1.565493	0.431190

2a	C	2.047569	-0.403503	1.625702
	H	2.703502	0.380206	1.997632
	H	1.030041	-0.210165	1.966446
	H	2.372850	-1.363026	2.023603
	C	2.071634	-0.447328	0.109070
	H	1.455607	-1.254152	-0.278206
	C	1.558559	0.823899	-0.530981
	O	0.693217	0.857205	-1.395984
	O	2.151194	1.928316	-0.030094
	H	1.768103	2.690555	-0.498887
	Cl	3.733991	-0.740381	-0.499341
	C	-1.992074	-0.039516	-0.234253
	H	-1.390798	0.265920	-1.081215
	Cl	-1.512509	-1.691029	0.186153
	Cl	-3.692725	0.035802	-0.692778
	Cl	-1.635153	1.078266	1.091967

2b	C	3.025844	1.655863	-0.510603
	H	3.023111	1.283461	-1.532441
	H	2.201925	2.360404	-0.384509
	H	3.962488	2.176482	-0.320515
	C	2.863124	0.510074	0.474189
	H	2.907036	0.857806	1.503126
	C	1.526304	-0.179903	0.315140
	O	0.681511	-0.230552	1.200762
	O	1.353271	-0.682789	-0.922078
	H	0.461518	-1.077290	-0.959857
	Cl	4.176246	-0.692128	0.280948
	C	-2.209432	-0.016380	0.239785
	H	-1.521531	-0.143619	1.066059
	Cl	-3.854660	0.043531	0.863885
	Cl	-1.990720	-1.418695	-0.832404
	Cl	-1.774857	1.480912	-0.589629

Cartesian coordinates (in Å) of S-(–)-2-chloropropionic acid monomers at the B3LYP/6-31++G level of theory combined with IEF-PCM solvent model for the $CHCl_3$ solvent.**

1	C	0.793079	1.735435	0.285224
	H	0.778189	1.972954	-0.776025
	H	0.124916	2.426905	0.802223
	H	1.800442	1.873097	0.672776
	C	0.328972	0.319945	0.532292
	H	0.358858	0.051572	1.586248
	C	-1.057728	0.030378	-0.025988
	O	-1.566202	0.639342	-0.935004
	O	-1.646825	-0.982356	0.619815
	H	-2.522927	-1.156151	0.206311
	Cl	1.457577	-0.878754	-0.277599

2	C	-0.618295	1.775360	0.005534
	H	-0.607802	1.800425	1.092928
	H	0.128032	2.479932	-0.368349
	H	-1.597050	2.091558	-0.350517
	C	-0.300050	0.387262	-0.515606
	H	-0.359168	0.335894	-1.599373
	C	1.076908	-0.119893	-0.115811
	O	1.897062	-0.497268	-0.919283
	O	1.286310	-0.074353	1.201689
	H	2.189143	-0.415045	1.392703
	Cl	-1.539500	-0.822127	0.078157

SQM B3LYP IR frequencies ($\tilde{\nu}$ in cm^{-1}). IR intensities (I_{IR} in km mol^{-1}). rotatory strengths (R_{VCD} in 10^{-44} esu^2 cm^2) and their robustness (ξ_{NB} in degree. ξ_{MG} in ppm)

	6-31++G**					**aug-cc-pVTZ**				
	1					**1**				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}		ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
617.6	37	-65	116.9	-27.4		619.0	31	-54	114.0	-26.9
662.3	122	121	77.1	13.9		662.0	98	110	75.4	15.8
778.7	8	-26	110.4	-57.5		789.9	8	-22	107.6	-48.9
808.8	9	-27	118.5	-58.1		809.1	9	-28	117.8	-61.2
981.9	15	4	67.5	14.0		983.5	13	3	73.2	11.3
1067.4	52	-49	163.0	-33.0		1067.1	68	-56	159.8	-29.8
1084.1	55	12	88.2	1.6		1084.0	51	19	84.2	5.6
1143.7	192	127	76.8	17.8		1138.3	173	126	75.7	19.3
1235.3	17	-27	121.6	-53.9		**1224.5**	21	-11	102.4	-22.1
1281.7	7	23	23.2	98.4		**1288.5**	4	19	27.9	152.7
1372.0	59	-21	101.3	-12.9		**1372.8**	46	-35	106.9	-26.3
1389.0	4	-10	126.1	-53.4		**1389.0**	6	-3	103.1	-11.7
1452.4	9	6	51.2	22.6		**1449.7**	9	5	63.7	16.7
1455.2	9	1	83.4	7.7		**1453.7**	7	1	79.4	11.3
1765.6	299	11	88.9	1.7		**1766.1**	288	8	89.2	1.3
2929.3	11	2	84.8	15.2		2934.5	10	2	85.3	15.7
2996.7	1	-6	135.4	-487.2		2997.2	4	-5	102.0	-82.2
3002.2	12	4	82.8	25.4		3004.6	7	4	75.6	48.9
3030.3	6	-4	102.8	-55.5		3028.7	5	-5	106.8	-75.0
3574.4	77	-5	92.1	-6.2		3573.3	78	-5	92.1	-5.9

2					**2**				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
596.8	49	-50	107.3	-18.2	599.9	46	-38	104.6	-15.2
685.0	78	-60	104.2	-12.7	687.6	64	-51	104.7	-13.7
776.1	8	21	77.4	41.9	787.3	9	18	79.2	35.0
808.9	5	6	67.6	25.7	808.4	5	6	63.7	32.3
966.3	29	20	28.1	18.0	967.5	28	24	30.6	21.0
1044.8	89	-127	144.9	-40.0	1043.8	89	-133	141.3	-40.7
1083.9	2	9	38.9	178.0	1084.5	2	9	43.5	181.5
1171.5	148	81	82.3	14.5	1170.8	145	96	80.8	17.2
1256.2	25	-38	152.8	-50.4	**1242.7**	22	-48	158.2	-67.8
1313.0	3	8	72.2	85.3	**1317.1**	2	5	74.0	100.5
1337.6	51	19	65.3	11.2	**1339.2**	39	20	69.7	16.4
1386.0	9	4	58.0	18.3	**1386.8**	6	3	63.8	15.5
1454.0	13	4	70.2	9.5	**1451.4**	13	4	72.9	10.4
1461.8	7	-1	96.0	-5.3	**1459.7**	5	0	84.3	4.7
1759.9	338	-21	92.4	-2.7	**1758.9**	330	-17	92.0	-2.3
2924.0	12	1	87.8	6.4	2930.1	10	1	87.8	7.1
2996.0	9	-2	93.8	-17.2	2995.3	8	-2	93.8	-18.8
3015.6	3	5	65.2	161.1	3016.1	3	5	71.1	123.9
3031.6	6	-2	98.9	-30.6	3033.3	5	-2	100.6	-37.1
3580.8	83	2	88.3	2.8	3578.2	83	3	88.3	2.9

3					**3**				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
602.4	71	86	73.3	17.4	609.2	58	68	74.4	17.4
689.9	50	25	75.1	4.5	692.6	46	24	78.4	3.7
736.6	5	3	76.7	51.7	747.9	5	5	77.9	46.1
815.1	2	5	49.0	56.5	817.1	2	4	53.2	49.9
965.0	35	-14	134.0	-9.8	965.2	35	-13	132.8	-9.1
1066.2	16	-35	107.8	-47.2	1067.2	11	-30	109.9	-65.6
1074.0	8	8	56.4	46.4	1075.9	12	5	52.1	29.5
1176.6	1	9	81.9	119.5	1180.2	3	14	77.0	172.7
1236.8	34	-14	115.1	-16.3	**1226.4**	28	-11	109.0	-14.5
1287.2	21	-7	95.6	-11.2	**1292.0**	11	-10	97.8	-20.9
1328.5	384	21	86.0	2.1	**1330.8**	365	14	87.1	1.5
1379.7	15	5	64.5	11.3	**1380.8**	16	6	63.5	12.7
1457.3	16	-12	166.4	-27.6	**1454.0**	15	-10	152.8	-24.5
1462.1	4	1	85.3	5.2	**1460.5**	3	0	93.0	-3.1
1779.5	281	-70	95.6	-11.2	**1776.9**	286	-69	95.3	-10.7
2934.3	8	1	81.6	9.8	2940.8	7	1	78.0	14.8
2997.8	3	5	68.2	142.9	2998.7	4	5	72.3	115.7
3015.0	6	2	84.8	22.4	3013.7	5	1	86.0	19.5
3019.4	7	-5	102.3	-53.8	3018.7	5	-4	103.4	-61.4
3514.1	134	-10	90.9	-7.2	3504.6	139	-8	90.7	-5.2

SQM B3LYP IR frequencies (ν in cm^{-1}). IR intensities (I_{IR} in km mol^{-1}). rotatory strengths (R_{VCD} in 10^{-44} esu^2 cm^2) and their robustness (ξ_{NB} in degree. ξ_{MG} in ppm)

	6-31++G**				aug-cc-pVTZ				
	1-1					1-1			
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
624.9	15	-24	179.9	-11.2	628.8	14	-12	112.4	-4.7
632.7	12	-21	127.8	-33.3	636.7	13	-9	135.3	-20.1
664.9	21	44	0.4	44.8	669.5	21	22	29.6	24.7
677.5	49	11	82.6	1.8	681.0	47	5	85.5	0.8
778.2	2	-6	9.2	69.4	788.0	2	-11	81.0	51.5
780.6	1	-13	152.9	-274.2	793.9	2	-2	146.2	-94.0
839.2	3	-12	179.9	-91.5	839.9	3	-7	169.0	-57.5
848.6	8	-4	98.3	-1.6	849.7	9	0	86.9	1.9
970.4	3	12	34.6	1598.7	958.3	4	3	34.8	767.3
982.1	6	4	10.1	52.8	984.1	2	2	98.2	-40.5
983.8	2	-13	113.4	-398.7	985.1	2	-6	120.4	-188.6
1016.4	202	-61	173.9	-6.8	1000.3	165	-16	95.8	-2.2
1074.2	37	-105	131.0	-76.6	1075.6	32	-50	118.5	-43.5
1075.0	24	118	2.4	146.2	1076.0	19	48	40.6	83.8
1094.3	12	4	91.1	-2.4	1094.7	12	4	89.9	0.2
1094.4	1	13	12.2	428.6	1094.7	2	3	44.2	228.6
1219.8	31	-98	175.9	-89.0	**1207.2**	27	-43	129.6	-45.9
1223.7	144	117	59.3	26.4	**1210.5**	108	35	70.9	9.7
1265.6	10	36	2.2	137.9	**1259.7**	4	11	38.5	171.0
1270.5	164	70	70.4	13.7	**1266.9**	225	67	61.4	8.9
1348.9	133	16	65.5	5.7	**1350.2**	12	-33	85.5	2.2
1349.1	11	-56	177.4	-440.1	**1351.2**	124	4	164.4	-198.8
1386.3	16	-16	106.3	-25.1	**1387.6**	11	-1	90.5	-0.9
1386.4	5	17	67.5	61.3	**1387.7**	10	1	87.9	0.1
1435.3	77	3	85.5	1.5	**1439.1**	38	5	89.0	1.8
1451.5	3	-39	178.7	-909.6	**1449.1**	3	-14	154.2	-257.8
1453.5	13	38	45.8	94.5	**1451.4**	14	14	63.5	23.8
1455.5	4	12	0.9	166.4	**1454.2**	3	3	49.2	95.4
1458.7	65	-14	97.9	-6.2	**1458.2**	70	-8	92.7	-2.1
1474.3	2	-15	177.6	4743.6	**1478.4**	1	-4	171.0	4170.2
1662.9	6	176	0.5	1416.2	**1661.0**	6	89	2.3	634.0
1716.5	706	-92	170.9	-6.0	**1714.0**	678	-43	92.7	-2.9
2901.5	1	-1	65.8	5315.1	2913.4	1	-1	34.1	274.2
2926.5	13	-10	99.3	-95.5	2931.8	10	-8	89.8	1.5
2926.6	17	4	167.6	-244.6	2931.9	16	1	136.5	3385.1
2997.6	147	-87	105.8	-80.0	2996.3	37	-1	97.2	-5.8
2997.8	6	0	95.8	-16.2	2996.5	19	-22	103.5	-85.1
3004.8	3047	43	106.7	-26.9	3008.5	379	-14	95.3	-5.6
3007.3	5	14	20.6	267.9	3009.1	10	0	67.4	78.7
3007.9	824	137	56.9	3.7	3014.5	3559	96	32.7	20.7
3031.3	3	-24	169.3	-732.1	3029.7	4	4	87.4	10.1
3031.3	5	6	125.5	-47.2	3029.8	5	-15	89.5	1.0

1-2					1-2				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
628.2	13	-20	109.0	-10.8	632.8	13	-1	83.0	1.0
641.6	9	16	52.5	30.1	645.1	8	16	33.8	37.0
670.0	5	12	102.8	-33.4	674.0	5	-1	110.6	-34.1
678.0	73	-4	89.3	0.2	681.6	70	-15	103.2	-3.9
777.7	2	-1	75.9	37.0	788.0	2	2	70.2	64.4
778.5	1	-5	130.3	-243.3	791.7	0	0	113.5	-60.7
839.3	1	-1	142.8	-11.5	840.1	1	0	87.4	3.1
847.9	11	-12	120.6	-17.0	848.9	12	-2	158.3	-3.5
970.7	0	-8	96.3	-52.6	959.7	0	-2	95.9	-20.3
974.1	7	22	66.1	76.4	976.4	5	21	49.1	140.6
982.8	3	-1	72.2	292.2	984.5	2	-1	120.5	-59.1
1015.6	203	-43	106.1	-5.6	1000.3	166	-18	100.8	-2.8
1063.5	45	-25	100.2	-16.1	1063.7	41	-41	105.9	-27.2
1074.5	30	-7	92.5	-5.5	1075.8	25	-4	125.1	-4.9
1088.6	1	9	53.4	195.0	1089.7	1	8	57.9	177.3
1094.3	7	9	75.7	47.4	1094.6	7	0	68.0	1.2
1221.9	86	-8	91.9	-2.3	**1209.1**	68	-15	136.9	-6.3
1251.3	29	9	87.6	5.0	**1235.8**	23	11	84.0	12.4
1268.3	64	57	62.9	24.5	**1263.8**	80	16	59.8	5.5
1307.2	172	-13	98.3	-7.1	**1301.9**	189	-28	110.4	-5.3
1312.6	18	32	82.4	4.5	**1317.9**	18	32	52.7	55.6
1349.0	75	-15	93.9	-6.2	**1350.6**	72	-8	102.7	-4.1
1383.5	6	2	85.0	10.2	**1385.1**	5	7	70.7	50.5
1386.5	10	3	86.1	8.3	**1387.7**	10	0	88.9	0.1
1432.0	82	0	85.1	3.5	**1436.1**	48	24	76.2	16.4
1452.0	9	-8	122.4	-319.7	**1449.8**	9	2	119.4	-49.4
1453.2	14	-8	94.0	-9.2	**1450.6**	16	-9	91.8	-3.9
1455.4	5	28	20.9	310.9	**1454.3**	5	8	40.3	141.5
1461.0	56	-51	106.3	-38.4	**1460.5**	57	-2	104.8	-8.7
1475.0	3	42	65.0	281.1	**1478.3**	1	13	52.9	449.9
1659.1	4	50	74.4	404.4	**1657.2**	4	24	76.9	192.4
1713.9	759	-29	97.6	-1.8	**1711.4**	735	-51	92.7	-3.2
2888.5	4	-44	95.0	-465.6	2899.8	1	-12	84.1	387.1
2924.3	14	0	98.3	-60.0	2930.1	12	0	100.9	-87.9
2927.0	15	1	96.7	-40.6	2932.4	12	-6	137.8	-87.4
2994.4	3702	-155	105.5	-53.8	2995.2	91	-32	99.1	-42.1
2996.7	267	104	105.6	-59.3	2996.8	114	24	60.9	12.0
2998.4	164	99	100.3	-8.1	3002.7	3863	349	73.6	21.9
3008.1	11	18	85.3	3.1	3010.7	52	-4	79.3	35.4
3016.1	0	5	85.4	9.6	3016.7	3	0	85.3	6.7
3031.4	4	-8	120.9	-216.9	3030.2	4	3	77.7	21.0
3032.9	5	-13	129.3	-181.6	3033.4	5	-11	144.5	-37.0

2-2					2-2				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
634.7	0	8	0.9	222.4	638.3	1	6	41.8	56.9
650.8	17	24	43.2	31.2	653.3	14	12	36.3	19.0
673.7	31	-72	179.8	-42.7	677.1	31	-39	152.2	-24.6
679.9	50	44	51.1	9.3	683.4	48	23	80.0	3.4
775.8	2	0	174.0	-30.1	785.7	1	0	94.5	-15.0
778.2	1	5	35.7	650.4	791.9	0	0	57.8	248.5
839.4	4	-12	179.8	-91.5	840.4	3	-5	178.8	-41.7
848.4	9	0	74.5	1.2	849.7	11	0	81.4	1.0
965.3	3	-21	160.8	-963.3	957.3	3	-8	163.6	-570.7
973.7	6	-17	176.6	-200.0	976.5	4	-9	113.1	-275.7
974.3	8	60	19.5	245.3	976.8	7	29	20.9	134.0
1012.3	200	-20	170.8	-3.4	1000.2	160	-9	95.6	-2.4
1063.2	60	-166	138.7	-74.3	1063.6	58	-80	129.9	-37.2
1063.8	21	86	2.2	117.9	1063.8	17	38	59.2	64.1
1088.6	2	8	83.9	31.0	1089.9	1	8	93.1	-9.8
1088.7	1	9	3.1	303.2	1090.1	2	-1	39.7	193.5
1252.0	32	10	54.9	84.1	**1236.1**	25	-30	111.4	-33.4
1252.1	32	-6	156.4	-71.0	**1236.4**	22	32	52.7	46.0
1301.9	10	51	9.3	125.3	**1296.8**	11	36	21.0	126.0
1311.9	43	2	44.6	76.9	**1309.3**	304	-50	122.0	-4.8
1312.8	109	-11	51.4	414.8	**1317.7**	40	36	52.9	33.3
1313.1	179	-12	136.7	-6.0	**1318.6**	1	-2	159.6	-697.5
1382.6	6	-9	128.9	-96.3	**1384.7**	6	-3	103.6	-27.3
1383.9	5	19	1.3	153.0	**1385.6**	3	7	48.0	80.7
1428.8	82	28	60.3	11.3	**1434.5**	49	9	85.7	5.6
1452.9	1	-14	179.0	1537.4	**1450.2**	3	-7	136.0	-74.1
1453.1	28	30	144.6	-461.5	**1450.4**	26	14	74.0	19.7
1455.3	3	-44	52.0	39.8	**1455.1**	2	-12	164.7	-459.3
1464.1	51	-16	102.6	-12.6	**1462.7**	50	-4	94.9	-4.4
1475.3	3	62	2.9	1095.7	**1478.6**	2	20	8.2	798.1
1655.1	2	-105	178.6	2986.4	**1652.9**	3	-68	175.5	1094.9
1710.5	812	54	77.6	3.0	**1707.4**	795	44	87.8	2.4
2885.1	1	-34	100.9	2941.8	2886.2	0	-8	94.8	1972.0
2923.7	10	12	83.7	82.0	2929.7	8	8	79.3	82.5
2923.8	21	-10	126.1	-83.3	2929.8	19	-6	102.0	-53.3
2991.7	4084	-32	102.7	-41.6	2990.9	4057	-29	99.8	-31.7
2996.2	5	-3	120.3	-71.6	2995.1	19	13	93.8	-6.0
2996.4	111	115	79.1	2.6	2995.4	136	51	89.3	1.4
3015.8	1	6	64.4	163.2	3016.5	1	4	22.8	644.2
3015.8	0	6	80.2	19.8	3016.5	0	0	89.5	0.9
3032.6	2	-17	172.5	-841.4	3033.3	3	-4	123.7	-153.9
3032.6	8	-3	132.0	-97.9	3033.4	6	-4	131.1	-58.4

SQM B3LYP/ aug-cc-pVTZ level IR frequencies (ν in cm^{-1}). IR intensities (I_{IR} in km mol^{-1}). rotatory strengths (R_{VCD} in 10^{-44} esu^2 cm^2) and their robustness (ξ_{NB} in degree. ξ_{MG} in ppm) of S-(–)-2-chloropropionic acid – $CHCl_3$ complexes

1a					1b				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
569.8	29	-11	98.5	-12.1	601.7	0	1	95.0	-3.8
621.4	27	-55	123.4	-30.0	640.7	23	-44	132.9	-18.8
665.7	91	118	69.0	19.4	665.0	18	-7	88.0	2.8
672.7	16	-9	82.0	11.1	690.4	76	76	78.5	12.4
747.4	153	22	87.5	3.0	732.1	166	-11	91.2	-1.2
751.3	158	-19	92.5	-2.8	767.6	155	4	89.9	0.2
788.3	10	-23	107.4	-40.9	791.6	16	-23	105.3	-25.2
812.6	9	-23	118.1	-45.7	818.5	8	-21	127.1	-52.8
984.5	13	8	73.6	21.2	983.6	13	4	82.3	11.8
1069.5	59	-60	140.6	-33.6	1071.8	26	-31	110.0	-34.7
1086.0	46	12	85.1	3.5	1088.8	31	-4	93.9	-5.4
1144.9	184	123	57.4	17.9	1159.0	172	74	38.3	11.7
1225.6	23	-8	106.1	-15.1	**1229.1**	20	26	33.1	91.2
1243.2	24	1	89.6	1.1	**1246.2**	31	-2	94.7	-10.2
1244.2	24	-6	93.6	-9.2	**1253.8**	24	1	89.4	1.8
1290.7	3	19	39.9	198.5	**1303.6**	2	12	9.0	208.5
1378.2	50	-36	99.5	-24.6	**1386.0**	58	-28	99.4	-25.1
1391.4	6	-3	107.5	-13.3	**1388.8**	5	-21	141.5	-41.8
1450.2	12	4	78.8	9.9	**1449.4**	9	6	71.5	19.3
1455.4	9	7	57.0	35.7	**1454.1**	9	0	84.3	6.9
1755.1	420	1	89.9	0.2	**1741.8**	294	25	80.7	3.9
2935.1	7	0	89.3	3.1	2934.1	9	3	85.2	26.9
2998.9	5	-6	105.0	-94.4	2997.9	6	-4	97.2	-51.8
3007.0	5	4	44.8	57.8	3007.2	6	3	76.2	36.8
3030.2	5	-4	107.8	-62.7	3029.8	6	-5	102.1	-69.5
3080.8	102	-5	92.1	-3.9	3054.6	111	9	87.4	6.5
3569.5	77	-5	90.9	-5.8	3460.6	455	-42	91.6	-8.4

2a					2b				
ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}	ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
577.0	67	64	74.7	20.3	615.8	27	-12	104.2	-6.9
603.7	45	-21	102.8	-9.0	633.2	18	51	29.2	72.0
671.4	20	5	85.7	3.9	664.6	18	10	84.8	8.7
688.9	61	-78	114.8	-23.1	695.5	69	-58	127.5	-13.9
743.3	162	8	89.1	0.9	731.3	168	7	89.5	0.4
755.2	156	2	89.5	0.6	767.9	153	-4	90.2	-0.2
786.5	10	13	81.1	27.9	790.4	16	14	83.1	14.1
813.0	5	5	69.6	23.1	818.4	6	3	65.7	13.6
970.8	24	19	71.3	19.4	971.0	20	15	74.3	18.6
1048.1	80	-120	153.2	-41.1	1050.5	66	-86	125.7	-35.3
1085.9	3	10	55.8	106.7	1086.3	1	7	49.7	211.7
1176.2	162	92	77.8	14.9	1197.5	105	68	33.0	17.5
1245.0	20	-76	99.6	-29.2	**1242.3**	19	9	71.3	52.0
1249.3	17	33	88.8	3.5	**1247.8**	41	-60	168.0	-69.8
1250.8	29	0	114.1	-27.0	**1254.9**	23	-3	93.3	-10.7
1322.7	3	2	84.9	35.8	**1318.2**	5	13	66.5	96.3
1347.9	46	22	81.1	15.3	**1361.6**	39	26	79.7	20.4
1388.4	8	0	87.5	3.8	**1389.1**	12	2	85.3	6.1
1451.5	13	6	72.6	16.4	**1450.8**	13	2	85.5	5.7
1459.9	6	-1	90.8	-1.3	**1459.4**	7	3	80.5	15.2
1744.1	445	-13	90.9	-1.4	**1734.9**	338	-14	92.2	-1.9
2930.8	8	0	89.9	0.5	2930.1	10	2	87.9	12.9
2996.3	7	0	90.4	-2.5	2995.6	8	-2	93.3	-19.8
3016.5	3	3	83.7	69.0	3016.5	3	5	73.9	120.4
3033.0	2	0	87.7	16.3	3033.4	4	-3	99.4	-53.9
3068.6	116	7	88.5	4.5	3053.4	111	-5	91.0	-3.4
3574.6	89	2	89.7	1.6	3464.3	478	31	88.6	6.0

$CHCl_3$ at the
B3LYP / aug-cc-pVTZ level of theory

ν / cm^{-1}	I_{IR}	R_{VCD}	ξ_{NB} / °	ξ_{MG}
256.1	0	0	91.4	-5.1
256.1	0	0	92.9	-9.5
362.1	0	0	73.7	0.0
672.5	4	0	95.4	0.0
749.6	163	0	90.0	0.0
750.1	163	0	90.0	0.0
1209.0	21	0	90.0	0.0
1209.2	21	0	90.0	0.0
3046.6	1	0	88.4	0.0

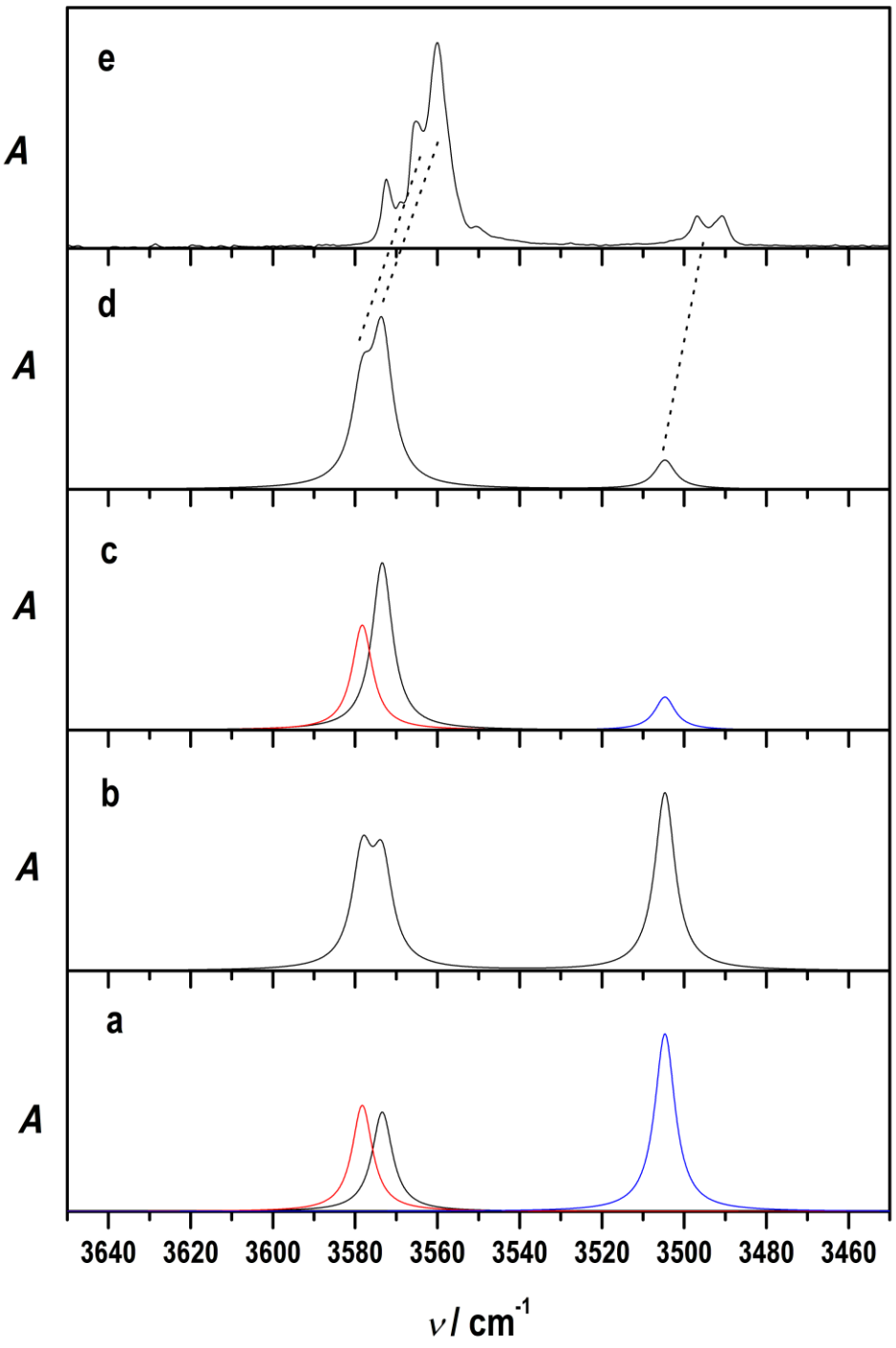
Calculated vibrational frequencies (unscaled. in cm) IR frequencies (unscaled. in cm^{-1}). IR intensities (I_{IR} in km mol^{-1}). rotatory strengths (R_{VCD} in 10^{-44} esu^2 cm^2) of S-(–)-2-chloropropionic acid – $CHCl_3$ complexes at the B3LYP / aug-cc-pVTZ level of theory combined with IEF-PCM solvent model for the $CHCl_3$ solvent.

1		
ν / cm^{-1}	I_{IR}	R_{VCD}
621.3	75	-56
639.6	153	148
786.6	12	-32
828.3	15	-26
1000.4	23	11
1084.3	1084	-64
1108.6	91	13
1161.4	267	157
1242.3	27	–35
1306.6	14	30
1397.8	79	–49
1416.6	8	–2
1480.5	12	2
1484.4	10	5
1774.7	484	–11
3039.2	7	1
3079.9	3	3
3079.9	9	-4
3133.7	5	5
3413.2	298	-17
2		
ν / cm^{-1}	I_{IR}	R_{VCD}
605.2	76	-48
662.1	107	-66
785.7	10	17
830.4	10	6
986.4	35	27
1062.9	116	-153
1104.1	3	12
1187.4	229	95
1262.7	29	–49
1340.6	3	10
1361.8	86	26
1413.1	7	3
1480.7	18	3
1489.5	7	–1
1764.3	547	–7
3033.8	7	0
3095.0	4	7
3103.2	9	-6
3132.1	4	0
3421.4	309	11

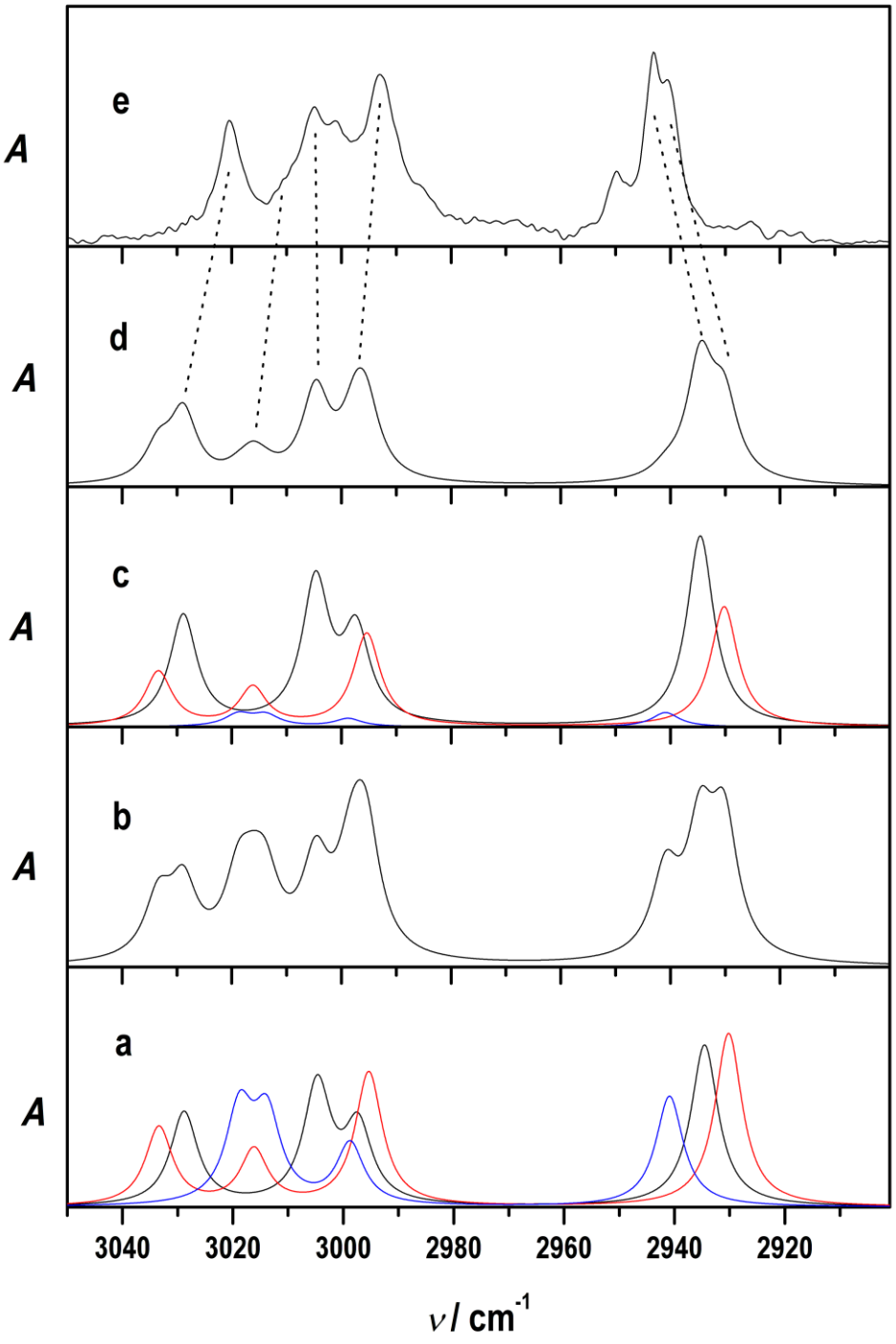
Assignment of the MI-IR and MI-VCD spectra of *S*-(–)-2-chloropropionic acid.

conformer	vibrational mode	ν / cm^{-1} calc.	ν / cm^{-1} exp.	VCD sign comp.	VCD sign exp.
2	ν_1	3578	3565.3572[a]		
1	ν_1	3573	3560.3550a		
3	ν_1	3505	3497. 3491[a]		
2	ν_2	3033	3023[b]		
1	ν_2	3029	3020		
2	ν_3	3016	3009sh		
1	ν_3	3005	3005.3001[a]		
1	ν_4	2997	2993		
2	ν_4	2995	2990[b]		
1	ν_5	2935	2943		
2	ν_5	2930	2941		
3	ν_6	1778	1791	-	not observable
1	ν_6	1766	1782	+	+
2	ν_6	1759	1773	-	-
2	ν_7	1460	1457	0	0
1	ν_7	1454	1453	+	-?[c]
2	ν_8	1451	1451[b]	+	-?[c]
1	ν_8	1450	1447	+	-?[c]
1	ν_9	1389	1388	-	-
2	ν_9	1387	1385	+	not observable
1	ν_{10}	1373	1380	-	-
2	ν_{10}	1339	1348	+	-?
3	ν_{10}	1331	1343	+	not observable
2	ν_{11}	1317	1324	+	not observable
1	ν_{11}	1289	1284	+	+
2	ν_{12}	1243	1259.1254[a]	-	-
1	ν_{12}	1225	1240.1233[a]	-	-
2	ν_{13}	1171	1181.1172[a]		
1	ν_{13}	1138	1148.1142[a]		
1	ν_{14}	1084	1094.1092[a]		
1	ν_{15}	1067	1073		
2	ν_{15}	1044	1046		
1	ν_{16}	984	997		
2	ν_{16}	968	985.980[a]		
1	ν_{17}	809	829.828[a]		
1	ν_{18}	790	778		
2	ν_{18}	787	775[b]		
2	ν_{19}	688	691		
1	ν_{19}	662	658		
1	ν_{20}	619	605		
2	ν_{20}	600	596		

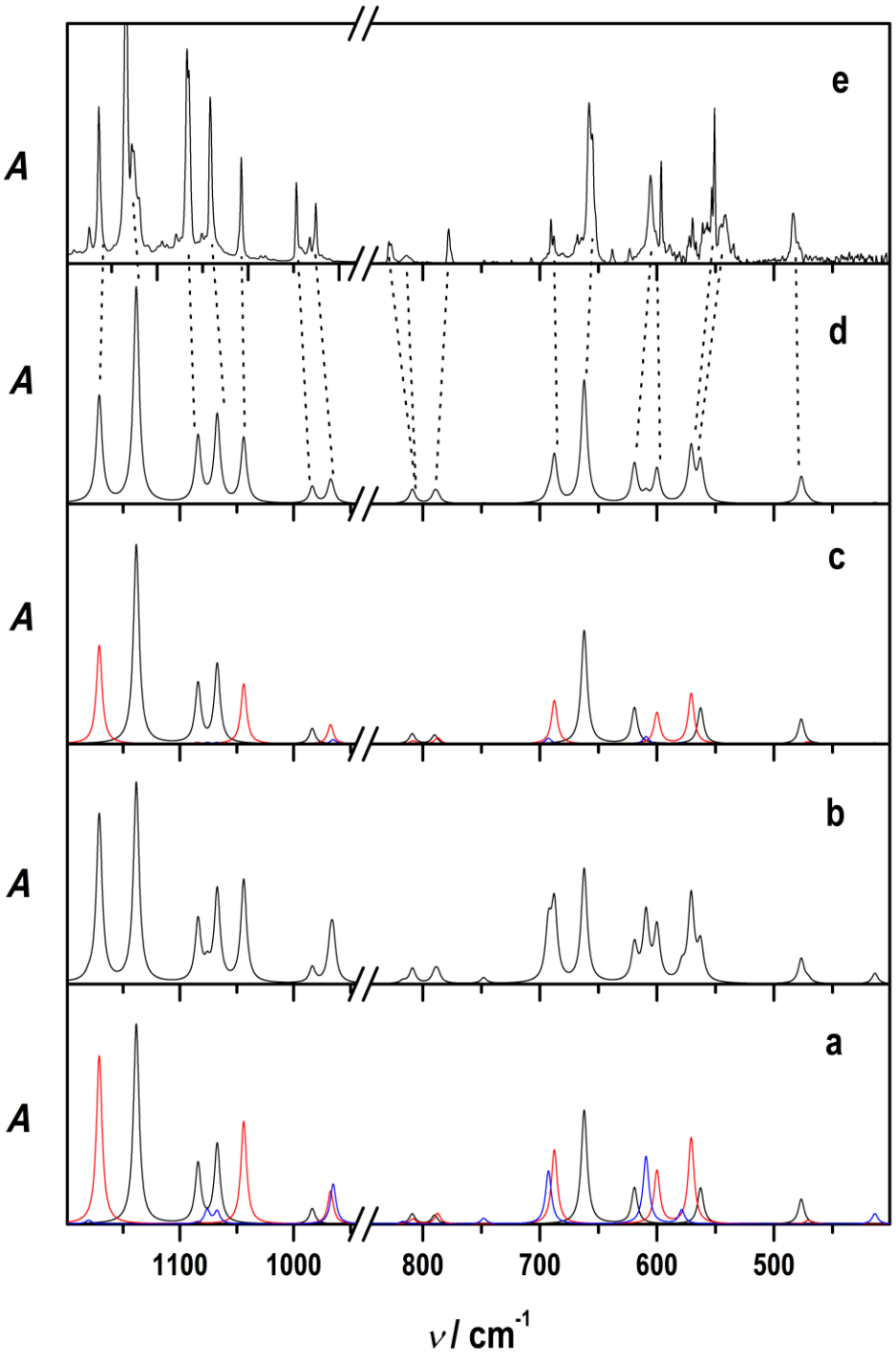
a: site splitting. b: shoulder. c: uncertain



a) Unweighted computed (B3LYP/aug-cc-pVTZ) IR spectra of the 3700-3400 cm^{-1} region of 2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line. b) Unweighted composite computed IR spectrum. c) Boltzmann-weighted computed IR spectra of2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line. d) Boltzmann-weighted composite computed IR spectrum. e) IR spectrum of 2-chloropropionic acid as observed in an 8 K Ar matrix.



a) Unweighted computed (B3LYP/aug-cc-pVTZ) IR spectra of the 3100-2900 cm^{-1} region of 2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line. b) Unweighted composite computed IR spectrum. c) Boltzmann-weighted computed IR spectra of 2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line.d) Boltzmann-weighted composite computed IR spectrum. e) IR spectrum of 2-chloropropionic acid as observed in an 8 K Ar matrix.



a) Unweighted computed (B3LYP/aug-cc-pVTZ) IR spectra of 1200-400 cm^{-1} region of 2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line. b) Unweighted composite computed IR spectrum. c) Boltzmann-weighted computed IR spectra of 2-chloropropionic acid conformers **1**: black line. **2**: red line. **3**: blue line. d) Boltzmann-weighted composite computed IR spectrum. e) IR spectrum of 2-chloropropionic acid as observed in an 8 K Ar matrix.