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NMR and parity violation: low-temperature dependence in ^{1}H CRAMPS and ^{13}C CP/MAS ssNMR spectra of alanine enantiomer

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Abstract

Life is based on L-amino acids and D-sugars rather than the enantiomeric D-amino acids and L-sugars. This broken symmetry is now believed to be a feature of fundamental physics—a result of symmetry-breaking induced by the weak force, which makes one enantiomer slightly more stable than the other. An amplification mechanism based on quantum mechanical tunneling could give rise to a second-order phase transition. In order to understand the transition mechanism, we measured the temperature dependence of ^{1}H CRAMPS solid state NMR and ^{13}C CP/MAS spectra of D- and L-alanine crystals from 295 K through to 220 K. Obvious difference of NMR behaviors between two enantiomers was observed in the phase transition which may be related to one suggested by Salam, caused biochirality among twenty amino acids.

Keywords: Parity violation; Alanine enantiomer; ^{1}H-CRAMPS-ssNMR; ^{13}C-CP/MAS-ssNMR; Phase transition; Parity-violating energy difference

1. Introduction

Chirality is a central feature of most theories of the origin of life. All biomolecules have to be of one hand, so homochirality is a hallmark of life. We argue that the weak force is the only universal truly chiral influence, which is one of the four forces of nature. The electromagnetic and weak forces were unified in 1968 by Salam and Weinberg. The world is made of fermions, which interact by exchange of virtual bosons. For example, the electrostatic repulsion between two electrons is mediated by exchange of virtual photons, while the weak interaction between an electron and a neutron is mediated by virtual Z^{0} bosons [1].

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Fermions exist in two states of opposite chirality, which are interconverted by parity (P). Parity is violated, since the weak force treats mirror images unequally. A left-handed electron participates in the weak interaction preferentially compared with a right-handed electron. This suggests that left- and right-handed electrons are not true mirror images but a left-handed electron and a right-handed positron are true images. A true mirror is not parity (P) but parity and charge conjugation (CP). Therefore, in strict speaking, L- and D-amino acid molecules are really diastereoisomers not enantiomers, owing to the handedness of their constituent elementary particles. The true enantiomer of an L-amino acid is the D-amino acid made of anti-matter. We argued that L- and D- alanine should differ in many properties, e.g. NMR chemical shifts [2].

In molecules the weak interactions include short-range parity-violating forces, which only take place in the nuclei. As the NMR chemical shift can be described as the modification of the external applied magnetic field B_0 due to the electron motion at the nucleus. One may expect that the chemical shift will be parity non-conservation (PNC) sensitive. Due to the weak interactions, a nucleus is chiral in itself, and thus the corresponding nuclei of a molecule, which exists in two enantiomeric forms, D and L, respectively, are in a diastereomeric environment and may exhibit NMR resonance frequency differences [3]. The contribution of the spin-dependent PNC terms, which usually play a minor role in the PNC experiments, the search for a parity-violating energy difference (PVED) in the two enantiomers spectra appears to be a challenge in molecules. Therefore, it requires an amplification mechanism of the PVED.

In 1991, Salam [4,5] suggested a unique mechanism whereby the PVED between enantiomers might lead directly to a homochiral product. He proposed that the subtle energy difference of chiral molecules induced by Z^0 interactions combined with Bose condensation may cause biochirality among twenty amino acids. It makes up proteins to be a consequence of second order phase transition below a critical temperature T_c, which is analogous to that of BCS superconductivity. The T_c for BCS superconductivity for metals is one of the form $\omega\exp[-2/g_{\text{eff}}\ \sigma(0)]$. Salam conjectured that a similar formula might be held for the case of amino acids chains. A crucial form for the transition temperature T_c involves dynamical symmetry breaking. The idea is supposed to start from the Feynman Lagrangian methodology of the BCS theory for the superconducting electronic system. The value of temperature T_c is deduced from the Ginberg–Landau equation. By using Sakita's formulation, the following result is presented.

$$T_c = \frac{\langle\varphi\rangle}{10^3}\exp\left[\frac{-2}{g_{\text{eff}}\sigma(1-4\sin^2\theta)}\right] \approx 2.5\times 10^2\ \text{K}$$

where the φ field is expressed as a complex auxiliary Higgs scalar field, g_{eff} is an attractive coupling constant between spin up ($\uparrow$) and spin down ($\downarrow$) electrons. The sign of g_{eff} is part of the assumption of the Hamiltonian which signifies an attractive force between Cooper-paired systems of electrons consist of one of the particles being replaced by its antiparticle with a factor of two which appears in the mass term. θ is the Weinberg angle. Salam took $(1-4\sin^2\theta)\approx 1/13$, with the empirical value of the parameter $\sin^2\theta \approx 0.231$, The exponential factor gives $\exp(-26)\approx 10^{-10}$. Assuming that $\sigma(0)=m_z^2$, we obtain $g_{\text{eff}}\sigma(0)\approx 1$. The theoretical phase transition temperature T_c is calculated to be approximately 250 K.

The present paper is to test the existence of Salam phase transition by low temperature dependence of ^{1}H CRAMPS ssNMR and the amplification mechanism of the phase transition which leads to the PVEDs of the D- and L-alanine crystals.

2. Experimental

2.1. Characterization of samples

The powder of D- and L-alanine were obtained from Sigma Chemical Corporation. The single crystals, were grown by slow evaporation of saturated aqueous solutions at 4 °C, then washed with absolute alcohol, evacuated and kept in a desiccator.

The characterization of D- and L-alanine single crystal was performed by the element analysis (C, H and N) and showed a good agreement between

the theoretical and experimental data. By using X-ray crystallography at 293 K, the cell dimensions of D- and L-alanine were determined as the same space group $P2_12_12_1$, orthorhombic, $a=0.60250$ nm, $b=1.2331$ nm, $c=0.57840$ nm, $V=0.42972$ nm^3. The data agree with Simpson [6] at 298 K, $a=0.6032$ nm, $b=1.2343$ nm, $c=0.5784$ nm, $V=0.4306$ nm^3. It indicated that D- and L-alanine are pure single crystals containing no crystalline H_2O molecule. The rotation angle ζ of the D- and L-alanine solution was measured on Polarimeter PE-241MC at 293K with the wavelength of 589.6 nm, respectively. By using the formula of $[\alpha]=\zeta/(L\times C)$, the corresponding α of D- and L-alanine were shown to be the same value but opposite sign.

2.2. Low-temperature dependence of ^{1}H solid state NMR spectra of D- and L-alanine

In previous studies we found the parity-violating effects in phase transition of D- and L-alanine single crystals at approximately 250 K by specific heat, DC-magnetic susceptibility and Raman spectroscopic properties [7]. In order to understand the transition mechanism, we want to know the low temperature dependence of α-proton ^{1}H-MAS ssNMR bands originating from the C–H fragment of D-alanine.

2.2.1. ^{1}H-MAS (magic-angle spinning) ssNMR spectra of D-alanine [8]

D-Alanine crystals were finely ground and packed in a 4-mm rotor sample tube, and then the sample was measured by Bruker DRX 300 WB from 220 K to 290 K. The sample amount was 94.9 mg. The chemical shift anisotropy of the nuclei is averaged out by magic-angle spinning (MAS). All the ^{1}H-MAS spectra were externally referenced to tetramethylsilane (TMS) with the chemical shift value of the methyl resonance assigned as zero. The spectrum of D-alanine shows three main peaks at 4.7720, 3.4085 and 0.9099, respectively, at 290 K. The signals were assigned to the NH_3^+, α-CH and the CH_3 group going from low to high magnetic field and the chemical shift values are coincident with those observed in the echo-MAS spectra [9,10]. The temperature dependence of the ^{1}H-MAS spectra of D-alanine from 290 K to 220 K were shown in Fig. 1 by single pulse excitation with a delay time of 4.5 μs at a spinning speed of 5 kHz with 256 scans. The results on D-alanine acquired at various temperatures imply that there exists a considerable difference between the surrounding electrical environment of the spin change which contribute to the high-resolution spectral component ^{1}H-αC. The peak of ^{1}H-αC showed an obvious upshielding under the decrease of the temperature. The integral peak area ratio of NH_3^+, α-CH and the CH_3 group in D-alanine was gradually moved from 3:1:3 to 3:0:4. It is coincident with the prediction by Salam [11] and confirmed the amplification mechanism of the phase transition. The shielding effect of metallic hydrogen is higher than the hydrogen of α-carbon in D-alanine molecule.

However, there is no the same phenomenon in L-alanine. Since the high-resolution echo-MAS method measures only a fraction of the solid which is usually small at room temperature and quite different from the majority of the solid in both molecular motion and chemical environment. For comparison, the CRAMPS technique was employed because it is quite efficient in removing the homonuclear dipolar interactions, which measures the proton system as a whole [10].

2.2.2. ^{1}H CRAMPS (combined rotation and multiple-pulse spectroscopy) ssNMR spectra of D- and L-alanine

The ^{1}H CRAMPS ssNMR spectra were run on a Varian InfinityPlus-400 spectrometer with resonance frequencies 400.12 MHz ^{1}H of D- and L-alanine. A 4-mm chemagnetics double probe was used for the variable temperatures ^{1}H CRAMPS experiments. A BR-24 multiple sequence was employed with a $\pi/2$ pulse width of 1.6 μs and 64 scans with a 2 s recycle delay to acquire CRAMPS spectra. The MAS rate was 2.5 kHz for the CRAMPS experiment. The amount of polycrystalline alanine sample was 26.8 mg. Chemical shifts were externally referenced to TMS. For the sake of investigating the temperature-dependent proton nucleus dynamics of D- and L-alanine molecules, the chemical shifts and peak widths of α-

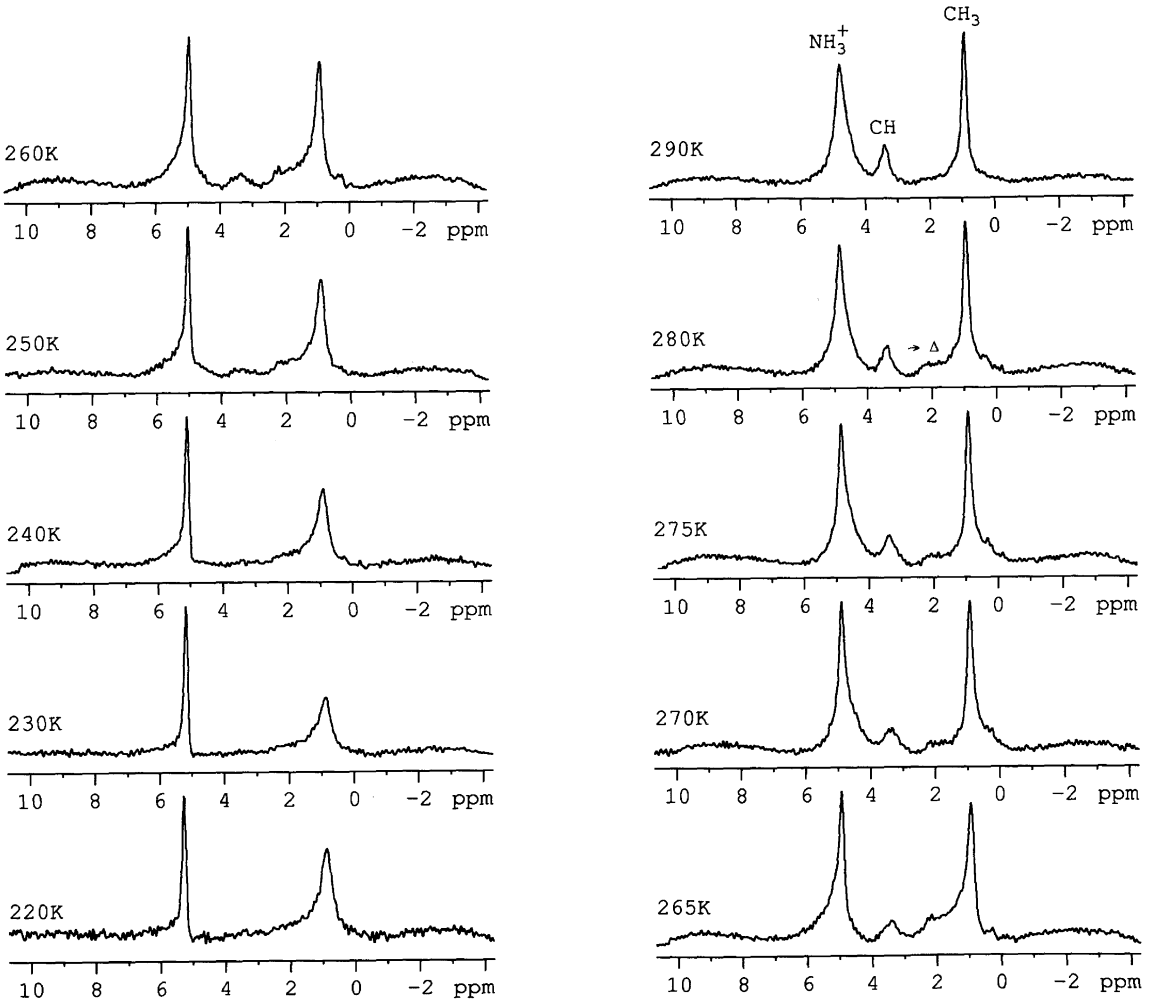

Fig. 1. Temperature dependence of ^{1}H-MAS spectroscopy of D-alanine.

H and β-H of D- and L-alanine were measured. The data are shown in Table 1 and Table 2.

Fig. 2 displays that four peak's widths of α-H and β-H experience distinct maximum at approximately 240 K. Therefore we conjecture that both D- and L-alanine may undergo a phase transition in this temperature range. In the L-alanine case, the variation degrees of peak widths of α-H and β-H peaks make a good agreement (the peak width is approximately two times as large as that in room temperature) in the whole process. It indicates the temperature-dependent spin–spin relaxation effects of α-H of and β-H nuclei of L-alanine molecule are nearly the same in the transition process. While in the case of D-alanine, the values of β-H peak width agree with those of L-alanine, however, the variation of α-H peak width is much fiercer (the peak width of D- is approx. 1.6 times as large as that in L- sample) than that of its enantiomer in the transition process.

From the above data, the peak linewidth represent spin–spin relaxation times T_2. The half height linewidth is given by $\Delta_{1/2}=1/\pi T_2$. $R_2=T_2^{-1}$ is the sum of several contributions, which corresponding to the different mechanisms, namely quadrupolar R_2^{Q}, dipolar interaction R_2^{D}, chemical

Table 1
Temperature dependence of the ^{1}H CRAMPS data of D-alanine

Temperature (K)	Peak	Freq. (ppm)	Freq. (Hz)	Position (Virt)	Intensity	Width $\Delta_{1/2}$ (Hz)	Integral	%Gauss
296	NH_3^+	8.687	1390.38	0.2821	356	390.87	23.623	0.0
α-H (C-H)		3.700	592.25	0.3741	798	84.43	11.998	0.0
β-H (CH_3)		1.142	182.71	0.4212	2905	100.76	51.499	0.0
280	NH_3^+	8.370	1339.65	0.2810	201	485.38	16.281	0.0
α-H (C-H)		3.685	589.72	0.3674	618	139.37	15.161	0.0
β-H (CH_3)		1.155	184.90	0.4141	2701	113.07	49.839	23.0
270	NH_3^+	8.759	1401.89	0.2735	117	872.31	15.144	23.0
α-H (C-H)		3.757	601.29	0.3657	448	204.93	14.885	23.0
β-H (CH_3)		1.225	196.05	0.4124	2237	128.14	46.63	23.0
265	NH_3^+	8.797	1407.96	0.2726	80	881.26	10.467	23.0
α-H (C-H)		3.736	597.88	0.3659	3788	239.74	14.584	23.0
β-H (CH_3)		1.203	192.58	0.4126	1973	138.70	44.388	23.0
260	NH_3^+	8.7981	1405.32	0.2728	57	925.37	7.810	23.0
α-H (C-H)		3.759	601.69	0.3654	335	249.39	13.422	23.0
β-H (CH_3)		1.232	197.13	0.4120	1813	147.31	43.251	23.0
255	NH_3^+	8.974	1436.29	0.2693	40	987.73	5.799	23.0
α-H (C-H)		3.610	577.84	0.3682	284	292.79	13.274	23.0
β-H (CH_3)		1.087	173.97	0.4147	1587	157.62	40.359	23.0
250								
α-H (C-H)		3.759	601.69	0.3654	335	249.39	13.422	23.0
β-H (CH_3)		1.232	197.13	0.4120	1813	147.31	43.251	23.0
240								
α-H (C-H)		3.510	561.84	0.3700	178	402.19	11.240	23.0
β-H (CH_3)		0.977	159.55	0.4163	1071	186.97	32.151	23.0
230								
α-H (C-H)		3.633	581.49	0.3673	150	373.31	8.824	23.0
β-H (CH_3)		1.125	180.03	0.4135	864	193.90	26.885	23.0
220								
α-H (C-H)		3.671	587.51	0.3666	134	344.21	7.325	23.0
β-H (CH_3)		1.142	182.79	0.4132	719	192.73	22.266	23.0
200								
α-H (C-H)		3.608	577.47	0.3678	123	248.88	4.940	23.0
β-H (CH_3)		1.056	1869.02	0.4148	444	185.62	13.250	23.0

shift anisotropy R_2^{CSA} and spin–spin coupling (*J*-coupling) R_2^J. In the CRAMPS experiment, the dipolar interaction R_2^D and the chemical shift anisotropy R_2^{CSA} are averaged out to zero. By choosing a spin 1/2 nucleus (^{1}H), the nuclear quadrupole moment is equal to zero, thus R_2^Q cancels out. The *J*-coupling R_2^J might be the predominant contribution. This part of study indicates the obvious difference *J*-coupling R_2^J values between D- and L-alanine in the phase transition process.

2.3. Low-temperature dependence of ^{13}C-CP/MAS (cross polarization and magnetic angle spinning) ss NMR of D-/L-alanine

2.3.1. ^{13}C-CP/MAS ssNMR of D-and L-alanine

The sample was measured by Bruker DRX 300 WB spectrometer with a 300 MHz, 89-mm magnet equipped with a CP/MAS accessory from 220 K to 290 K. The ^{13}C chemical shifts were calibrated through the external adamantine peak. The

Table 2
Temperature dependence of the ^{1}H CRAMPS data of L-alanine

Temperature (K)	Peak	Freq. (ppm)	Freq. (Hz)	Position (Virt)	Intensity	Width $\Delta_{1/2}$ (Hz)	Integral	%Gauss
295								
α-H (C-H)		3.763	602.33	0.3729	773	122.41	16.654	0.0
β-H (CH_3)		1.202	192.43	0.4202	2882	108.00	54.599	0.0
280								
α-H (C-H)		3.912	626.11	0.3702	623	164.56	17.889	0.0
β-H (CH_3)		1.348	215.76	0.4175	2902	106.10	54.045	0.0
270								
α-H (C-H)		3.921	627.54	0.3700	476	185.48	15.304	0.0
β-H (CH_3)		1.340	214.43	0.4176	2448	120.23	51.441	0.0
265								
α-H (C-H)		3.955	632.95	0.3694	403	194.82	13.585	0.0
β-H (CH_3)		1.376	220.28	0.4170	2258	126.85	49.960	0.0
260								
α-H (C-H)		3.844	615.30	0.3714	341	216.87	12.726	0.0
β-H (CH_3)		1.252	220.34	0.4192	2027	136.69	48.147	0.0
250								
α-H (C-H)		3.795	607.44	0.3724	284	233.04	11.343	0.0
β-H (CH_3)		1.192	190.82	0.4203	1769	148.11	45.341	0.0
240								
α-H (C-H)		3.933	629.41	0.3698	169	253.97	7.321	0.0
β-H (CH_3)		1.300	208.00	0.4184	1177	181.38	36.590	0.0
230								
α-H (C-H)		3.982	637.26	0.3689	133	261.19	5.934	0.0
β-H (CH_3)		1.340	214.44	0.4176	924	195.23	30.782	0.0
220								
α-H (C-H)		4.103	656.61	0.3667	123	242.48	5.089	0.0
β-H (CH_3)		1.470	235.32	0.4152	765	192.58	25.193	0.0
200								
α-H (C-H)		3.665	586.54	0.3748	126	195.01	4.239	0.0
β-H (CH_3)		1.084	173.46	0.4223	519	177.96	15.800	0.0

obtained polycrystalline samples were ground by agate mortar before the NMR measurements in order to eliminate the orientation anisotropy of crystals in the spinning rotor. The spinning speed is 5 kHz. Spectra were usually accumulated 256 times to achieve a reasonable signal-to-noise ratio. The spectra of D-/L-alanine show three main peaks at 280 K as 139.385/139.393 ppm, 12.464/12.880, 12.403 ppm and −17.956/−17.961 ppm which were assigned to be the carbonyl group (COO^-), α-carbon (C–H) and β-carbon (CH_3 group), respectively. We compared our results with Ye et al. [12] and Asaka et al. [13] and found a good agreement. The dynamic behavior of α-C signals changed greatly with a decrease in temperature as shown in Fig. 3. The splitting of α-C of D-alanine at 265 K implied the coexistence of an intermediate and a quick decrease then disappearance of the α-C peak below 260 K, which may be related to a phase transition which happened from D-alanine ↔ intermediate ↔ L-alanine (Table 3).

2.3.2. ^{13}C CP/MAS ssNMR spectra of D- and L-alanine measured on a Varian Infinity Plus-400 spectrometer

The ^{13}C CP/MAS ssNMR spectra of D- and L-alanine were obtained on a Varian InfinityPlus-400 spectrometer with resonance frequencies 100.62

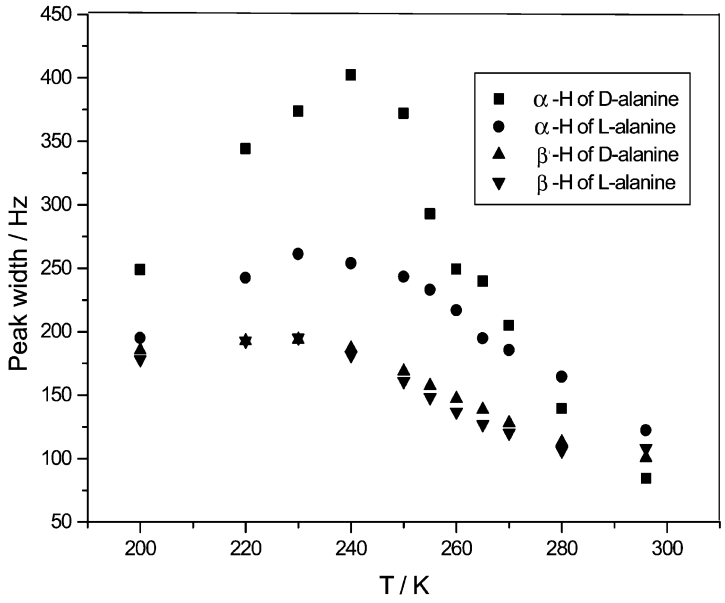

Fig. 2. Temperature dependence of peak width of α-H and β-H in D- and L-alanine.

MHz for ^{13}C. A 4-mm Chemagnetics double probe was used for the variable temperatures ^{13}C CP-MAS experiments. It was performed with a 3 s recycle delay, 256 scans and a contact time of 2.5 ms. The MAS rate was 5 kHz. The sample amount was 45 mg. Chemical shifts were referenced to HMB (hexamethylbenzene) for ^{13}C measurement. The data are shown in Table 4.

The spectra of D-/L-alanine show three peaks at 250 K as 178.036/177.992 ppm, 51.167/51.015 ppm and 20.634/20.586 ppm, which was assigned to be the carbonyl group (COO^-), α-carbon (C–H) and β-carbon (CH_3), respectively. In comparing the temperature dependence data of ^{13}C-ssNMR of D-and L-alanine, the difference is worthy to notice. The chemical shifts change in a crystal due to the surrounding electron environment of the spin change. A variation in chemical shift may happen due to the varied shielding effect. We proposed that the upfield of α-carbon of D-alanine presents α-C electron-shielding increase from the lengthening of bond distance of C–H under temperature decrease and the downfield of carbonyl of L-alanine represents electron-deshielding increase by the decrease of the electronic density.

3. Results and discussion

A method for calculating the NMR chemical shift tensor components has been developed by Ramsey. To the parity-conservation terms which enter in the molecular Hamiltonian, the neutral current PNC terms of the electron–nucleon interaction are added. There are essentially two static NMR parameters, namely the magnetic shielding tensor σ and the indirect spin–spin coupling tensor *J*. The corresponding Hamiltonian, written in frequency units for a nucleus *i* is

$$H_i = (1/2\pi)\gamma_i I_i(1-\sigma)B_0$$

There is no first order contribution to σ. Here γ_i is nuclear magnetogyric ratio, I_i is spin number operator. *J* is the indirect spin–spin coupling.

In general, the resonance frequencies and the spin–spin couplings of the corresponding nuclei in both isomers are identical. However, if PNC is taken into account, the NMR spectra of two enantiomers will show differences, expected to be small according to the prefactors existing in the σ_{PNC} and J_{PNC} matrix elements. Considering the case of σ for a nucleus alone, it comes for the D and L enantiomers:

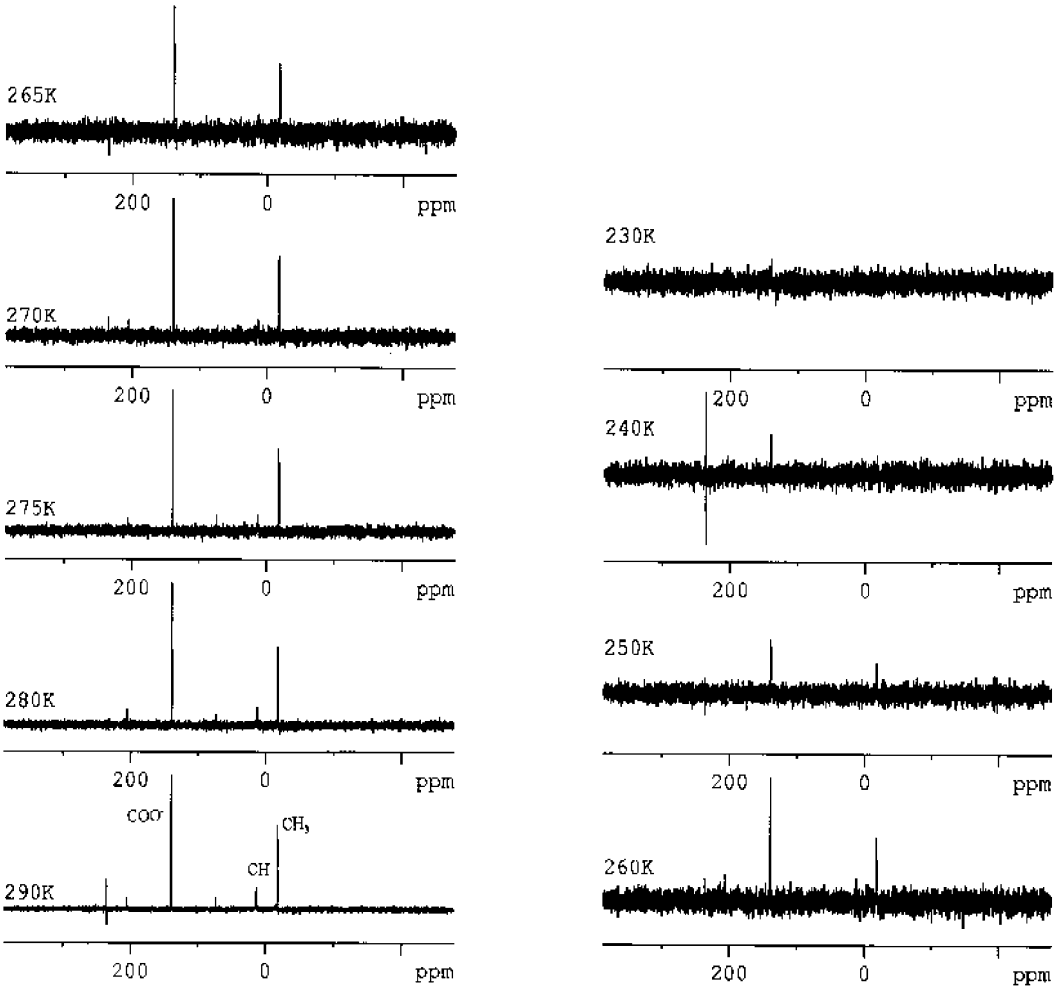

Fig. 3. Temperature dependence of ^{13}C-CP/MAS spectra of D-alanine.

Table 3
Comparison of the chemical shift of α-C and β-C in D- and L-alanine (calibrated with external adamantine peak)

Sample	T/K	290	280	275	270	265	260	250
D-Ala (ppm)	α-C	12.4638	12.4403	12.5454	12.6557	12.9691/ 12.5426	12.5869	–
	β-C	−17.9728	−17.9562	−17.9705	−17.9821	−18.0220/ −17.0262	−18.0215	−17.9827
L-Ala (ppm)	α-C	12.8797/ 12.4028	12.4708	12.7922/ 12.3160	12.5739/ 12.2574	–	–	–
	β-C	−17.9605	−17.9765	−17.9845	−18.0016	−17.9938	−18.0370	−17.9532

Table 4
Temperature dependence of the ^{13}C CP/MAS spectra of D- and L-alanine (calibrated by external HMB)

Temperature (K)	α-C-H		β-C(CH_3)		Carbonyl group (COO^-)	
	D-Alanine	L-Alanine	D-Alanine	L-Alanine	D-Alanine	L-Alanine
299	51.401	51.228	20.819	20.677	178.166	177.968
280	51.187	51.145	20.652	20.661	177.996	178.005
275	51.166	–	20.650	–	178.002	–
270	51.134	51.085	20.659	20.607	177.991	177.968
265	51.103	51.113	20.653	20.606	178.041	177.977
260	51.169	51.158	20.641	20.627	178.009	178.004
255	–	51.053	–	20.589	–	177.967
250	51.167	51.015	20.634	20.586	178.036	177.992
240	51.073	51.042	20.628	20.580	178.068	178.023
230	51.159	51.015	20.602	20.554	178.068	178.023
220	51.097	51.002	20.591	20.548	178.070	178.078

$$\nu_D=(1-\sigma-\sigma_{PNC})\nu_0,\quad \nu_L=(1-\sigma+\sigma_{PNC})\nu_0,$$
$$\Delta\nu=2\sigma_{PNC}\gamma_N B$$

Thus a splitting in each line of a racemic mixture should be a clear cut manifestation of PNC at the molecular level. The NMR line splittings between the two enantiomers of Tl compounds have been calculated by Barra et al. At 11.7 T [$\nu(^1H)=500$ MHz], the frequency resonance differences, only a few mHz, lie below the best resolution now attainable for ^{13}C [2].

The internuclear indirect spin–spin coupling is different from the direct dipolar coupling. It corresponds to the internuclear coupling through the polarization of the bonding electrons. The corresponding Hamiltonian is, in frequency units, for two coupled nuclei i and j, $H_{ij}=J_{ij}I_i\times I_j$. The highest J_{ij} values may reach a few kHz [J(Pb–C) = 16.625 kHz; J(Tl–C) = 10.5 kHz; J(Sn–Sn) ≈ 15 kHz) [2,14,15]. Nuclear spin must be $1/2$ (^1H no quadrupolar moment), in order to avoid quadrupolar line broadening or splitting. Besides B_0 field inhomogeneity, the NMR linewidth is determined by the spin–spin relaxation time T_2:

$$\Delta\nu_{1/2}=(\pi T_2)^{-1}$$

The peak linewidth of NMR spectra is originated from the uncertainty principle:

$$\Delta E\times\Delta t\approx h$$

Here Δt is the time of the particle staying on a certain energy state. In the NMR phenomena, the staying time of nuclear magnetic moment Δt is decided by spin–spin interaction. T_2 is the interaction time constant, therefore:

$$\Delta E\times T_2\approx h,\quad \Delta E=h\Delta\nu,\quad \therefore\Delta\nu\approx 1/T_2$$

Because of the inhomogeneous of the magnetic field, $\therefore\Delta\nu\approx 1/T_2'$, T_2' is the apparent transverse relaxation time. $\therefore\Delta_{1/2}=1/\pi T_2'$

$$\therefore\Delta E_D=h\Delta\nu\approx h\times 1/T_2' h\times\pi\times\Delta_{1/2}$$

$\approx 6.626\times10^{-34}$ Js $\times 3.1416\times 402.19$ Hz (the highest $\Delta_{1/2}$ value of α-H of D-alanine)
$\approx 1\times 3.1416\times 402.19$ Hz
≈ 1.263 kHz
$\approx 5.216\times10^{-12}$ eV

$$\Delta E_L=h\Delta\nu$$

$\approx 6.626\times10^{-34}$ Js $\times 3.1416\times 253.97$ Hz (the $\Delta_{1/2}$ value of α-H of L-alanine at 240 K)
$\approx 5.286\times10^{-31}$ J
$\approx 3.299\times10^{-12}$ eV
$\approx \Delta\nu_L\approx 0.798$ kHz

Calculation of the PVED between mirror image molecules have been reported for light molecules [16,17] and lie in the range 10^{-15}–10^{-20} eV. The effect of the PNC contribution to the spin–spin coupling between electrons S_1DS_2 in the triplet state of chiral molecules has been considered; a ratio of approximately 10^{-12}–10^{-13} eV with respect to the spin–orbit coupling has been estimated [18].

The simple physical description of σ and *J* clearly shows that their values are expected to be highly dependent upon the behavior of the electrons in the vicinity of the nuclei. These two quantities, which can be measured with a high accuracy in high resolution NMR experiments for the study of PNC in molecular physics. The present studies show the experimental evidence of parity violation in this phase transition. However, this cannot be simply interpreted as the configuration change of D→L because of the evident divergence of D- and L-enantiomers in the low-temperature physical properties of chemical shift. Had the D-sample transferred to L-, the low-temperature physical properties of them would have been the same.

The parity-violating low-temperature NMR behavior of D- and L-alanine, together with the characteristic of phase transition measured by specific heat, DC-magnetic susceptibility and Raman spectroscopy, provides a significant insight to the role of weak neutral current played in the low-temperature phase transition and physical properties of amino acids. We expect this phenomenon to be generally present in other amino acids. The fact that D- and L-alanine experience different behavior below T_c may be considerably important in the application of enantiomeric separation in low temperature. Further study may lead to clues for the understanding the origin of homochirality.

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