Supplementary Information for:

Identification of beryllium fluoride complexes in mechanically distorted gels using quadrupolar split ^{9}Be NMR spectra resolved with solution-state selective cross-polarization

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1. Quantum chemical calculations

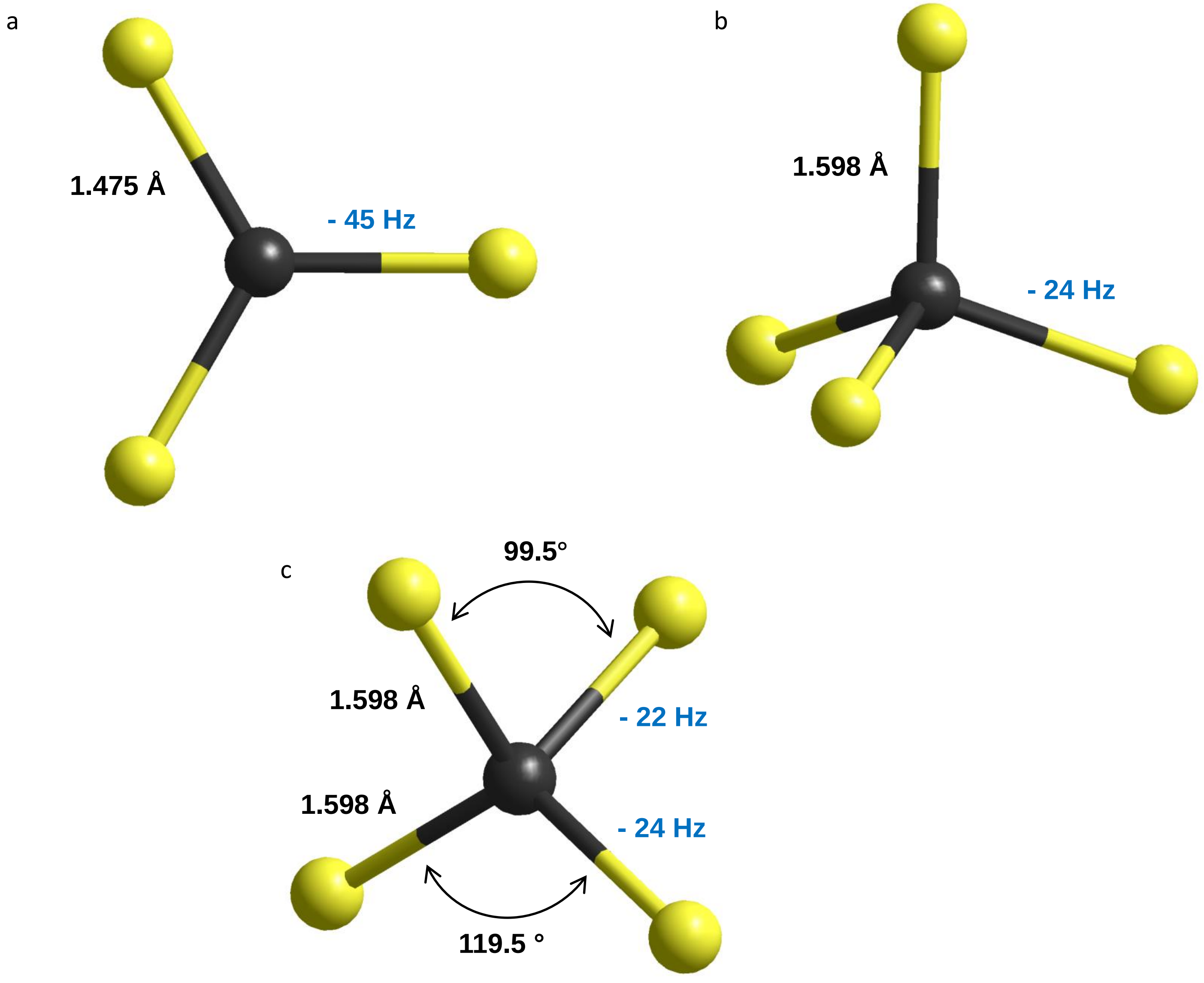


Fig. S.1. (a, b) BeF_3^- and BeF_4^{2-} structures calculated using GAUSSIAN program,[1] respectively. The *J*-coupling constants of BeF_3^- and BeF_4^{2-} "in vacuum" are -45 and -24 Hz, and the corresponding bond lengths are 1.475 Å and 1.598 Å, respectively. The parameters of quadrupolar interaction for ^{9}Be nucleus of the BeF_3^- complex are C_Q = -1.81 MHz and $\eta = 0$. For a perfect tetrahedral BeF_4^{2-} structure, $C_Q = 0$. (c) A distorted BeF_4^{2-} tetrahedron and corresponding *J*-coupling constants. The parameters of quadrupolar interaction are C_Q = 159 kHz and $\eta = 0.9$.

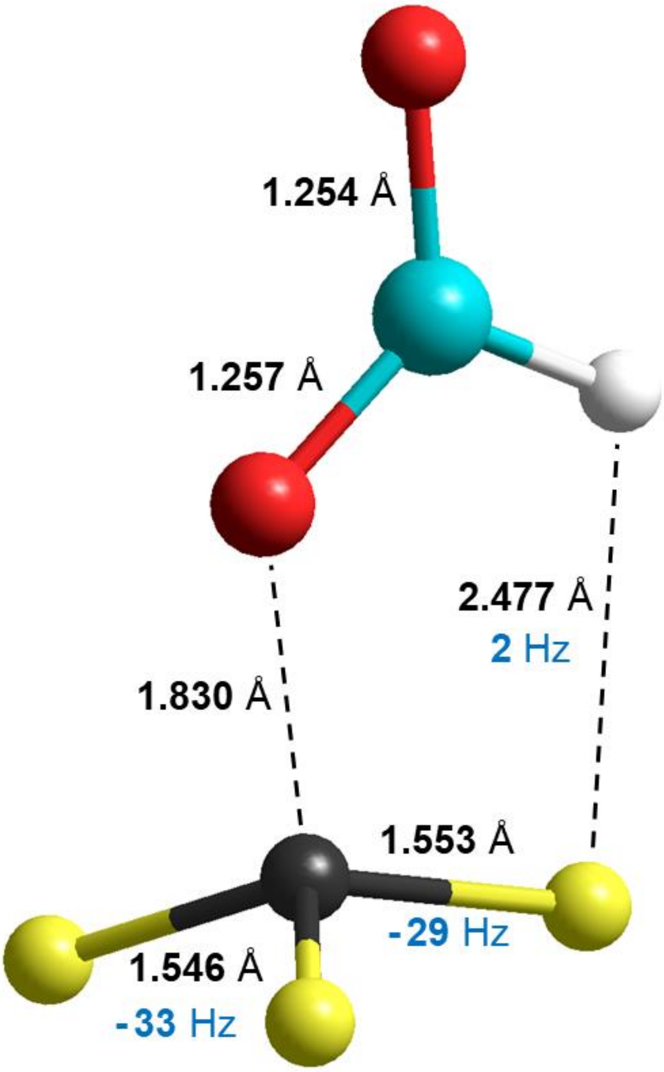


Fig. S.2. A structure of the (BeF_3^- $COOH^-$) complex and associated *J*-coupling constants calculated using GAUSSIAN program.[1] Atoms are coloured as follows: Be – black, F – yellow, C – cyan, O – red, H – white. The parameters of quadrupolar interaction are C_Q = - 732 kHz and η = 0.09.

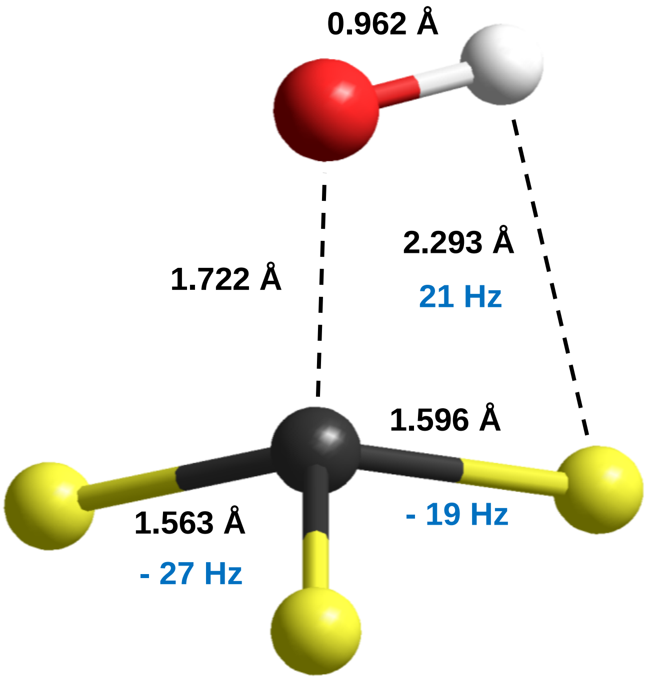


Fig. S.3. A structure of the (BeF_3^- OH^-) complex and associated *J*-coupling constants calculated using GAUSSIAN program.[1] Atoms are coloured as follows: Be – black, F – yellow, C – cyan, O – red, H – white. The parameters of quadrupolar interaction are C_Q = - 248 kHz and η = 0.63.

2. Dynamics of Cross-Polarization in Solution of J -Coupled Spin 1/2 -Spin 3/2 Nuclei

This mathematical/quantum mechanical analysis is an expansion of that presented in Eykyn *et al.*[2] and is given in a form that is readily implemented in the *Mathematica*-based NMR software package *SpinDynamica*. The spin density operator $\hat{\rho}(0)$ describes the state of a spin system at a time $t = 0$. To calculate the state of the spin system at $t = \tau$, we propagate the spin density operator $\hat{\rho}(0)$ forward under the action of a time-propagation operator (also called a propagator) $\hat{U}(\tau)$:

$$\hat{\rho}(\tau) = \hat{U}(\tau)\hat{\rho}(0)\hat{U}^{-1}(\tau), \qquad \text{(A1)}$$

where the propagator $\hat{U}(\tau)$ is defined as:

$$\hat{U}(\tau) = exp\{-i\hat{H}\tau\}, \qquad \text{(A2)}$$

and where $\hat{H}$ is the Hamiltonian operator that describes all influences that act on the spin system between $t = 0$ and τ.

In the case where all the terms contained within $\hat{H}$ commute with each other, *i.e.*, $[\hat{H}_i, \hat{H}_{ii}] = 0$, diagonalization of the matrix form of $\hat{H}$, in a suitable basis, yields eigenvalues that provide physical insight into the dynamics of the spin system. The analytical form of $\hat{H}$ is also easily determined in this case and it is used to investigate the influences of radiofrequency (*rf*) pulse sequences acting on the spin system.

In cases where all the terms contained within $\hat{H}$ do *not* commute with each other, *i.e.*, $[\hat{H}_i, \hat{H}_{ii}] \neq 0$, it is possible to transform $\hat{H}$ into a frame of reference in which the non-commuting terms vanish. We assume that in such a frame, the rotating magnetic fields at the nutation frequencies of all *rf*-pulses are strong compared with the interaction strengths of the individual spins, *e.g.*, quadrupolar couplings, scalar couplings etc., and that all *rf*-pulses are on resonance. For the following discussion, we consider the case of heteronuclear polarization transfer in cross-polarization (CP) experiments conducted on solutions.

Consider a 2-spin system composed of the nuclear isotopes ^{9}Be ($I = 3/2$) and ^{19}F ($S = 1/2$) (as described in the main article). During the ‘contact’ *rf*-pulses of a CP experiment the Hamiltonian operator $\hat{H}$ that acts on the BeF spin system has the form:

$$\hat{H} = \hat{H}_Z + \hat{H}_J + \hat{H}_Q + \hat{H}_{RF}, \qquad \text{(A3)}$$

where $\hat{H}_Z$ is the Zeeman Hamiltonian operator, $\hat{H}_J$ is the scalar coupling Hamiltonian operator, $\hat{H}_Q$ is the quadrupolar Hamiltonian operator for the ^{9}Be spin, and $\hat{H}_{RF}$ is the *rf*-pulse Hamiltonian operator. These Hamiltonian operators have the following definitions:

$$\hat{H}_Z = \omega_0^I \hat{I}_Z + \omega_0^S \hat{S}_Z, \qquad \text{(A4)}$$
$$\hat{H}_J = 2\pi J_{IS} \hat{I}_Z \cdot \hat{S}_Z, \qquad \text{(A5)}$$
$$\hat{H}_Q = \frac{\omega_Q^I}{6}\left(2\hat{I}_Z \cdot \hat{I}_Z - \hat{I}_X \cdot \hat{I}_X - \hat{I}_Y \cdot \hat{I}_Y\right), \qquad \text{(A6)}$$
$$\hat{H}_{RF} = \omega_1^I \hat{I}_X \cos(\omega_0^I \tau) + \omega_1^S \hat{S}_X \cos(\omega_0^S \tau), \qquad \text{(A7)}$$

where ω_0^I and ω_0^S are the nuclear Larmor frequencies for spins *I* and *S*, respectively, J_{IS} is the scalar coupling constant, ω_Q^I is the quadrupolar coupling constant for spin *I*, and ω_1^I and ω_1^S are the respective nutation frequencies of the simultaneous *rf*-fields applied to spins *I* and *S* during the contact period. For spin *I*, the quadrupolar frequency ω_Q^I is:

$$\omega_Q^I = \frac{3e^2qQ}{2I(2I-1)\hbar}\,\frac{1}{2}\left(3\cos^2\theta - 1 + \eta\sin^2\theta\cos 2\varphi\right) \qquad \text{(A8)}$$

Here Q is the electric quadrupole moment of the ^{9}Be nucleus, eq is the electric field gradient (EFG) at the ^{9}Be nucleus, and $C_Q = \frac{e^2qQ}{h}$ is the quadrupole coupling constant (Hz). In Eqn (A8), the order of principal values of the nuclear quadrupole interaction tensor is defined as:

$$|Q_{XX}| \le |Q_{YY}| \le |Q_{ZZ}|, \qquad Q_{XX} + Q_{YY} + Q_{ZZ} = 0.$$

Here θ and φ are the second and third Euler angles, respectively, determining the orientation of the nuclear quadrupole interaction tensor in the laboratory frame system, in which with the external magnetic field B_0 is parallel to the *z* axis. In the following analysis, applicable to axially distorted gel samples, the EFG asymmetry parameter η is 0 and θ is also 0.

It should be apparent that all of the terms in the Hamiltonian operator $\widehat{H}$ do not all commute with each other, and as a result; we now perform a series of transformations which remove the contact CP *rf*-pulses from the expressions for the transformed Hamiltonian. At the end of this analysis, we will be left with a Hamiltonian operator in a new frame of reference in which the remaining terms commute with each other. In this new frame, it will be much easier to describe the dynamics of the contact CP *rf*-pulse sequence.

We first transform the Hamiltonian operator $\widehat{H}$ into a doubly rotating frame of reference. This frame precesses at a frequency ω_0^I for spin *I* and ω_0^S for spin *S*, *i.e.*, the *rf*-pulse frequencies of both spins about the axis of the static magnetic field B_0, which we assume to be the *z*-axis of the laboratory frame. This is accomplished mathematically by introducing the following transformation:

$$\widehat{H}^{dr} = \hat{R}_0 \widehat{H} \hat{R}_0^{-1} - \widehat{H}_Z, \qquad \text{(A9)}$$

where the superscript *dr* stands for 'doubling rotating'. The rotation operator $\hat{R}_0$ is defined as:

$$\hat{R}_0 = \exp\left(-i\omega_0^I \hat{I}_Z \tau\right) \exp\left(-i\omega_0^S \hat{S}_Z \tau\right). \qquad \text{(A10)}$$

With this transformation, the first exponential operator acts only on spin *I*, while the second one acts only on spin *S*. Furthermore, for this transformation to be valid, we assume that $\omega_Q^I \ll \omega_0^I$, *i.e.*, only small or residual quadrupolar coupling constants apply. The doubly rotating Hamiltonian operator $\widehat{H}^{dr}$ has the form:

$$\widehat{H}^{dr} = \widehat{H}_J + \widehat{H}_Q + \widehat{H}_{RF}^{dr}. \qquad \text{(A11)}$$

In the newly established doubly rotating frame, the scalar coupling Hamiltonian operator $\widehat{H}_J$ is invariant to the frame transformation, since $\hat{R}_0^{-1} \widehat{H}_J \hat{R}_0 = \widehat{H}_J$. Furthermore, the frame transformation simply interchanges the $\hat{I}_X$ and $\hat{I}_Y$ terms of the quadrupolar Hamiltonian operator $\widehat{H}_Q$ for spin *I* (Eq. A6), and as a result; this Hamiltonian operator is also invariant to the frame transformation. Meanwhile, the form of the *rf*-pulse Hamiltonian operator $\widehat{H}_{RF}$ (Eq. A7) has been influenced by the previous frame transformation. This Hamiltonian operator is also given the superscript *dr*. The form of the doubly rotating *rf*-pulse Hamiltonian operator $\widehat{H}_{RF}^{dr}$ is:

$$\hat{H}_{RF}^{dr} = \omega_1^I \hat{I}_X + \omega_1^S \hat{S}_X. \qquad \text{(A12)}$$

Note that the time dependence of the applied *rf*-field has been removed by the transformation into the doubly rotating frame as the *rf*-pulses are assumed to be on resonance. At this point in the analysis the doubly rotating *rf*-pulse Hamiltonian operator $\hat{H}_{RF}^{dr}$ is *tilted* by an angle $\pi/2$ about the -*y*-axis of the doubly rotating frame. The utility of this rotation of the spin operators will become clear below. This is performed mathematically by the operation:

$$\hat{H}^{drt} = \hat{R}_1 \hat{H}^{dr} \hat{R}_1^{-1} \qquad \text{(A13)}$$

where *drt* denotes the 'doubly rotating tilted' frame. The rotation operator $\hat{R}_1$ is defined as

$$\hat{R}_1 = \exp\,(i\pi\hat{I}_Y/2)\,\exp\,(i\pi\hat{S}_Y/2). \qquad \text{(A14)}$$

The doubly rotating tilted frame Hamiltonian operator $\hat{H}^{drt}$ has the form:

$$\hat{H}^{drt} = \hat{H}_J^{drt} + \hat{H}_Q^{drt} + \hat{H}_{RF}^{drt}. \qquad \text{(A15)}$$

The scalar coupling, quadrupolar and CP contact *rf*-pulse Hamiltonian operators in the doubly rotating tilted frame have the form:

$$\hat{H}_J^{drt} = 2\pi J_{IS} \hat{I}_X \cdot \hat{S}_X, \qquad \text{(A16)}$$
$$\hat{H}_Q^{drt} = \frac{\omega_Q^I}{6}(2\hat{I}_X \cdot \hat{I}_X - \hat{I}_Z \cdot \hat{I}_Z - \hat{I}_Y \cdot \hat{I}_Y), \qquad \text{(A17)}$$
$$\hat{H}_{RF}^{drt} = \omega_1^I \hat{I}_Z + \omega_1^S \hat{S}_Z. \qquad \text{(A18)}$$

We now transform into the frame of the contact CP *rf*-pulses. This frame is often called the 'interaction frame', since only terms related to the scalar coupling and quadrupolar interactions are left. This frame retains the effects of the CP contact *rf*-pulses and nullifies the influence of such *rf*-pulses in the doubly rotating tilted frame Hamiltonian operator $\hat{H}^{drt}$. The transformation used to achieve this is one which rotates the current doubly rotating tilted frame of reference about the new *z*-axis, the direction of the CP contact *rf*-pulses in this frame, at a precession rate of ω_1^I for spin *I* and ω_1^S for spin *S*:

$$\widehat{H}^{drtr} = \widehat{R}_2 \widehat{H}^{drt} \widehat{R}_2^{-1} - \widehat{H}_{RF}^{drt}, \qquad \text{(A19)}$$

where *drtr* denotes the ‘doubly rotating titled rotating’ frame of reference. The rotation operator $\widehat{R}_2$ is defined as:

$$\widehat{R}_2 = \exp\left(-i\omega_1^I \hat{I}_Z \tau\right) \exp\left(-i\omega_1^S \hat{S}_Z \tau\right). \qquad \text{(A20)}$$

This transformation is similar to the doubly rotating frame transformation described earlier, but it is around the new *z*-axis of the doubly rotating tilted frame of reference. The resulting total Hamiltonian operator $\widehat{H}^{drtr}$ in the doubly rotating titled rotating frame has the form:

$$\widehat{H}^{drtr} = \widehat{H}_J^{drtr} + \widehat{H}_Q^{drtr} \qquad \text{(A21)}$$

Clearly, whatever transformations have acted upon the CP contact *rf*-pulse Hamiltonian operator must have also acted upon the various interaction Hamiltonian operators. For the frame of the CP contact *rf*-pulses, a *SpinDynamica* calculation gives the new forms of the doubly rotating titled rotating scalar coupling and quadrupolar Hamiltonian operators, which remain active under the influence of the CP contact *rf*-pulses, as follows:

$$\widehat{H}_J^{drtr} = \frac{\pi J_{IS}}{2}\left(e^{i(\omega_1^I+\omega_1^S)\tau}\left(\hat{I}^- \cdot \hat{S}^-\right) + e^{i(\omega_1^I-\omega_1^S)\tau}\left(\hat{I}^- \cdot \hat{S}^+\right) + e^{-i(\omega_1^I-\omega_1^S)\tau}\left(\hat{I}^+ \cdot \hat{S}^-\right) + e^{-i(\omega_1^I+\omega_1^S)\tau}\left(\hat{I}^+ \cdot \hat{S}^+\right)\right), \qquad \text{(A22)}$$

and

$$\widehat{H}_Q^{drtr} = \frac{\omega_Q^I}{24}\left(3\left(e^{2i\omega_1^I\tau}\left(\hat{I}^- \cdot \hat{I}^-\right) + e^{-2i\omega_1^I\tau}\left(\hat{I}^+ \cdot \hat{I}^+\right)\right) + 2\left(\hat{I}_X \cdot \hat{I}_X + \hat{I}_Y \cdot \hat{I}_Y - 2\hat{I}_Z \cdot \hat{I}_Z\right)\right). \qquad \text{(A23)}$$

The doubly rotating tilted rotating frame is related to the laboratory frame by a rotation $\omega_0 t$ around the *z*-axis, a tilt through $\pi/2$ around the new -*y*-axis, and another rotation through $\omega_1 t$ around the new *z*-axis. Of course, ω_0 and ω_1 are related to the particular nuclear species of interest. In the doubly rotating titled rotating frame, the Hamiltonian operator $\widehat{H}^{drtr}$ has a complex time dependence on ω_1^I and ω_1^S. Consequently, a secular approximation is now required to remove any rapidly oscillating terms:

$$\widehat{H}_J^{sdrtr} = \frac{\pi J_{IS}}{2}\left(e^{-i(\omega_1^I-\omega_1^S)\tau}\left(\hat{I}^- \cdot \hat{S}^+\right) + e^{i(\omega_1^I-\omega_1^S)\tau}\left(\hat{I}^+ \cdot \hat{S}^-\right)\right), \qquad \text{(A24)}$$

and

$$\widehat{H}_Q^{sdrtr} = \frac{\omega_Q^I}{12}\left(\hat{I}_X \cdot \hat{I}_X + \hat{I}_Y \cdot \hat{I}_Y - 2\hat{I}_Z \cdot \hat{I}_Z\right), \qquad \text{(A25)}$$

where *sdrtr* denotes the ‘secularized doubly rotating titled rotating’ Hamiltonian operator. The non-secular terms are ignored by the secularization process since these terms oscillate at high frequencies, *i.e.*, ω_1^I or ω_1^S, and are assumed to average to zero over the course of the CP contact *rf*-pulses.

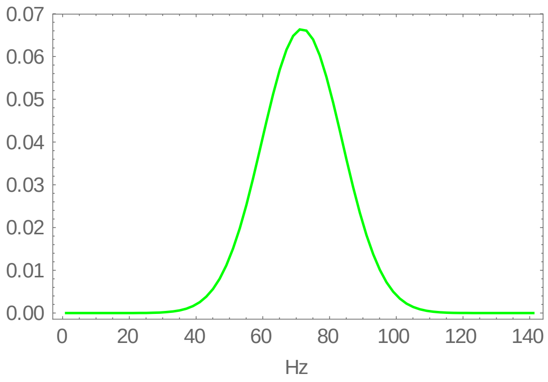
When $\omega_1^I \neq \omega_1^S$, the scalar coupling Hamiltonian operator $\widehat{H}_J^{sdrtr}$ is dampened, and it has little effect on the dynamics of the spin system since the oscillating terms average to zero throughout the CP contact period. At this point, the complicated time dependence may be further simplified by assuming that the two contact *rf*-pulses satisfy the Hartmann-Hahn condition, *viz.*, $\omega_1^I = \omega_1^S = \omega_1$, which is necessary for efficient CP outcomes. Hence,

$$\widehat{H}_J^{hhsdrtr} = \frac{\pi J_{IS}}{2}\left(\hat{I}^- \cdot \hat{S}^+ + \hat{I}^+ \cdot \hat{S}^-\right), \qquad \text{(A26)}$$

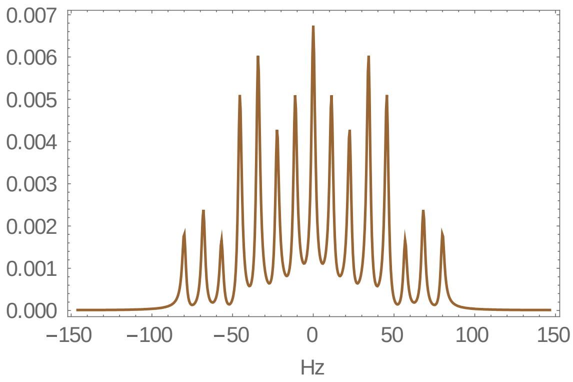
where *hhsdrtr* denotes the ‘Hartmann-Hahn secularized doubly rotating titled rotating’ Hamiltonian operator. This operator is uninfluenced by the strict Hartmann-Hahn matching condition, which is $\widehat{H}_Q^{sdrtr} = \widehat{H}_Q^{hhsdrtr}$. Clearly, the oscillating terms have disappeared from the scalar coupling Hamiltonian operator $\widehat{H}_J^{hhsdrtr}$ and they cause a double resonance effect between the *I* and *S* spins that constitutes nuclear polarization transfer. Now that the Hartmann-Hahn matched and secularized doubly rotating tilted rotating frame Hamiltonian operator $\widehat{H}^{hhsdrtr} = \widehat{H}_J^{hhsdrtr} + \widehat{H}_Q^{hhsdrtr}$ has been derived, it can be used to predict NMR spectra that result from IS nuclear polarization transfer that originates in CP experiments on solutions of heteronuclear *J*-coupled spin-½/spin>½ systems.

3. SpinDynamica code for simulation of a cross-polarization spectrum of the spin 3/2 nucleus (^{9}Be) *J*-coupled to four spins 1/2 (^{19}F).

```
$Path[];
AppendTo[$Path,"C:\\....\\SpinDynamica"];
Needs["SpinDynamica`"];
SetUserLevel[3];

(* The spin system corresponds to a BeF4 complex *)
SetSpinSystem[{{1, 3/2}, {2, 1/2}, {3, 1/2}, {4, 1/2}, {5, 1/2}}];

(* Initial density operator of the 19F spins after the first excitation RF pulse *)
ρini=NormalizeOperator[opI[{2,3,4,5},"x"]];
ρini//MatrixRepresentation//MatrixForm;
ρobs = NormalizeOperator[opI[1, "-"]];

(*Set up the doubly resonant radiofrequency fields*)
ωS=2π 88; (* γB1 for 19F, rad*Hz *)
ωI=2π 88; (* γB1 for 9Be, rad*Hz *)

drf=ωI opI[1,"x"]+ωS opI[{2,3,4,5},"x"];
PREP = {drf/.{ωI->2π 88, ωS->2π 88}, 0.0125};

(* Set up the parameters of the spectrum of the BeF4 quintet *)
LB = 2.8; (* Line broadening, Hz *)
W = 0.05; (* Central frequency of the quintet, Hz *)
J= -34.13; (* J-coupling constant, Hz *)
ωQ = 2*Pi*11.42; (* Mean Residual Quadrupolar Coupling, RQC, rad*Hz *)
ωQsigma = 2*Pi*2.25; (* HWHM of the distribution of RQCs *)

(* Averaging scheme for EnsembleAverage function, "Gaussian" distribution of RQCs *)
t = Range[ωQ-5*ωQsigma, ωQ+5*ωQsigma, 2]; (*list of RQC values*)
F = Gaussian[t, {ωQ, ωQsigma}]/Total[Gaussian[t, {ωQ, ωQsigma}]];
SCHEME = Transpose[{t, F}]; (* The averaging scheme used in the EnsembleAverage function below*)

(* Plot the distribution of RQCs *)
ListPlot[SCHEME, PlotStyle-> {Green}, FrameLabel-> {{None, None}, {HoldForm[Hz], None}}]
```

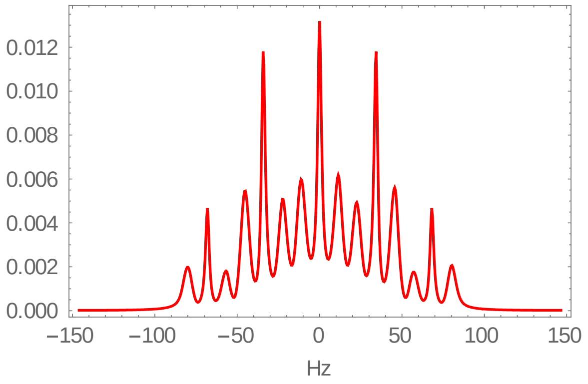


```
(* Create the total interaction Hamiltonian *)
H = 2π W opI[1,"z"] + (ωQ/Sqrt[6])opT[1,{2,0}] + 2π J opI[1, "z"].opI[{2, 3, 4, 5}, "z"];

(* CP spectrum of BeF4 without RQC distribution *)
pentet = Signal1D[{{2*Pi*292.96, 300}}, InitialDensityOperator -> ρini, Preparation -> PREP,
BackgroundGenerator -> H, Observable -> ρobs, LineBroadening -> 2*Pi*LB];
Expand[pentet];

ReV= Re@FT@pentet;
ListPlot[ReV, PlotStyle->{Brown}, FrameLabel->{{None,None}, {HoldForm[Hz], None}}]
```



```
(* CP Spectrum of BeF4 including the RQC distribution *)
ωQ =.;

(* Hamiltonian *)
H = 2π W opI[1,"z"]+(ωQ/Sqrt[6])opT[1,{2,0}] + 2π J opI[1, "z"].opI[{2, 3, 4, 5}, "z"];

(* Calculation of the time domain signal *)
pentet = Signal1D[{{2*Pi*292.96, 300}}, InitialDensityOperator -> ρini, Preparation -> PREP,
BackgroundGenerator -> H, EnsembleAverage-> {ωQ, SCHEME}, Observable -> ρobs,
LineBroadening -> 2*Pi*LB];
Expand[pentet];

RePentet= Re@FT@pentet; (* Fourier transform of the time domain signal *)

(* Normalizing the spectrum *)
RePentet[[;; , 2]]= RePentet[[;; , 2]]/Total[RePentet[[;; , 2]]];
```

```
SPECTRUM = RePentet;

(* Plot the CP spectrum *)
ListPlot[SPECTRUM, PlotStyle->{Red}, FrameLabel->{{None, None}, {HoldForm[Hz],
None}}]
```



4. *SpinDynamica* simulations of ^{9}Be CP-NMR spectra of BeF_4^{2-} and BeF_3^{-} complexes in mechanically distorted gels.

Figure S4 shows experimental and simulated ^{9}Be CP-NMR spectra of the BeF_4^{2-} complex in a Gelita gel subjected to different compression states. The quantum mechanical principles of the CP experiment are described in Appendix 1. The broadening of quadrupolar satellites was simulated with *SpinDynamica*, as described in Appendix 2, using Normal distributions of RQCs. The normal distributions were described with values of mean quadrupolar couplings (Q^{V}) and half width at half maxima (HWHM).

Figure S5 shows experimental and simulated ^{9}Be CP-NMR spectra of the BeF_3^{-} complex in a stretched *Sigma*-75 gel. Broadening of quadrupolar satellites was described using a bimodal distribution of RQCs comprised of two Gaussian functions. Parameters of the Gaussian functions were Q^{IV} (1) and HWHM (1) for the dominant, and Q^{IV} (2) and HWHM (2) for the secondary BeF_3^{-}components, respectively.

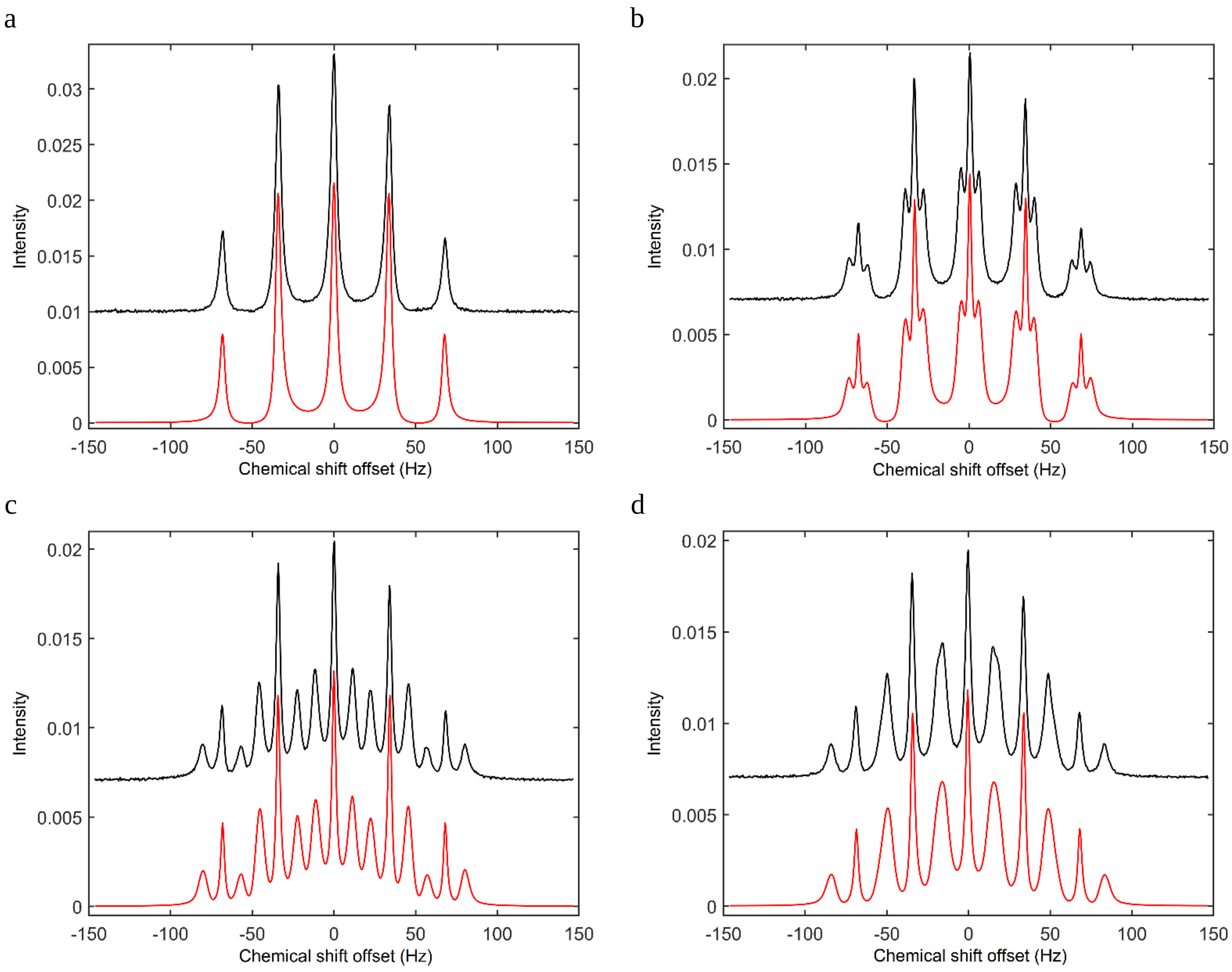


Fig. S.4. ^{9}Be CP-NMR spectra of BeF_4^{2-} (black) and *SpinDynamica* simulations (red) for a Gelita gel (76% BeF_4^{2-} and 24% BeF_3^{-}) at different states of mechanical distortion: (a) Relaxed; (b-d) compressed by factors of 1.2, 1.4 and 1.53, respectively. Parameters of the *SpinDynamica* simulations:

a. J^{V} = -33.95; LB = 4.

b. J^{V} = -34.1; Q^{V} = 5.67; HWHM = 1.95; LB = 2.8.

c. J^{V} = -34.1; Q^{V} = 11.42; HWHM = 2.25; LB = 2.8.

d. J^{V} = -34.1; Q^{V} = 14.86; HWHM = 2.7; LB = 3.1.

The CP contact time is 12.5 ms.

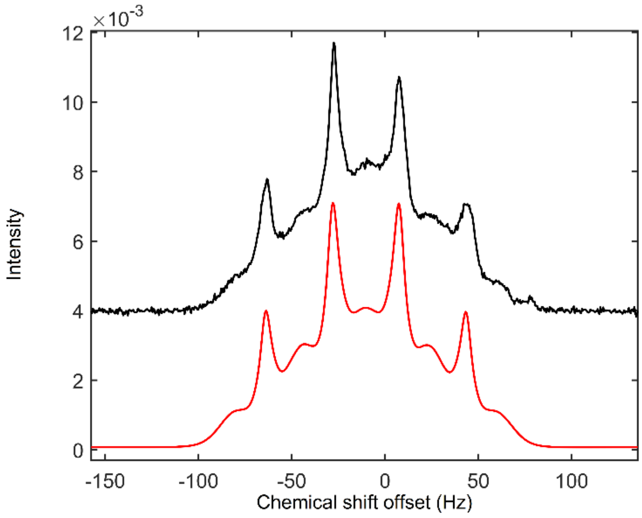


Fig. S.5. A *SpinDynamica* simulation (red) of the experimental CP-NMR spectrum (black) of BeF_3^- in the *Sigma*-75 gel stretched by a factor of 1.7.

Parameters of the *SpinDynamica* simulations (Hz):

J^{IV} =-35.9;

Q^{IV} (1) = 16;

Q^{IV} (2) = 4;

HWHM (1) = 8.5;

HWHM (2) = 2;

LB = 7.5.

The CP contact time is 11 ms.

Definitions:

J^{V} – *J*-coupling of the quintet (Hz)

J^{IV} – *J*-coupling of the quartet (Hz)

Q^{V} – mean RQC of the quintet (Hz)

Q^{IV} – mean RQC of the quartet (Hz)

HWHM – half-width at half-maximum of the Gaussian function (Hz)

LB – Inhomogeneous line broadening (Hz)

References

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