Experimental:

All syntheses were carried out under deoxygenated and dried argon or nitrogen by use of standard Schlenk techniques or an inert gas glove box. All solvents were dried prior to use.

Elemental analyses were carried out using a Perkin Elmer Series II CHNS/O analyzer 2400 and a Perkin Elmer 2380 Atomic Absorption Spectrophotometer (Ni). NMR spectra were acquired on a Bruker Avance 400 spectrometer. IR UV/Vis spectra were acquired with a DU 650 Beckman spectrophotometer.

The ligands were synthesized according to modified literature methods (Bz_3TAC, $(oFBz)_3TAC$).(see ref 1)

Synthesis of hexakis(acetonitrile)nickeltetrafluoroborate

$[(MeOH)_6Ni](BF_4)_2$ was obtained according to the literature method [(a) Drago, R. S.; Meek, D. W.; Longhi, R.; Joesten, M. D. *Inorg. Chem.* **1963**, 2, 1056-1060; (b) Wickenden, A. E.; Krause, R. A. *Inorg. Chem.* **1965**, 4, 404-407.] by adding 2,2-dimethoxypropane (5 ml, 40.7 mmol) (tri(ethyl)orthoformate can also be used) to hexaquonickeltetrafluoroborate (1 g, 2.94 mmol) (recrystallized from saturated solution in thf, commercial or prepared from mixing $Ba(OH)_2 + 2\ HBF_4$(aq) + $NiSO_4$(aq) after filtering off of $BaSO_4$). The resulting green solution was stirred extensively for two hours. After removing the volatile materials an other 1 ml of 2,2-dimethoxypropane was added, stirred for 15 minutes and then removed in vacuo. The raw $[(MeOH)_6Ni](BF_4)_2$ was obtained as a light green solid in almost quantitative yield: Anal. Calcd for $C_6H_{24}O_6B_2F_8Ni$: C, 16.97; H, 5.70. Found: C, 15.80; H, 5.16.

Acetonitrile (5 ml, 95.7 mmol) was added to raw $[(MeOH)_6Ni](BF_4)_2$ (1.25 g, 2.94 mmol) and stirred for 20 minutes. The volatile materials were removed in vacuo and the whole procedure was repeated two times. The blue $[(MeCN)_6Ni](BF_4)_2$ was recrystallized by cooling of saturated solutions in acetonitrile.

Anal. Calcd for $C_{12}H_{18}N_6B_2F_8Ni$ (6 MeCN): C, 30.11; H, 3.79; N, 17.56. Anal. Calcd for $C_{10}H_{15}N_5B_2F_8Ni$ (5 MeCN): C, 27.45; H, 3.46; N, 16.01. Found: C, 28.1; H, 3.74; N, 16.0. Apparently up to one eq is lost during drying in vacuo.

$[(MeCN)_4Zn](BF_4)_2$ was obtained in an analogous procedure resulting in colourless needles after recrystallisation from MeCN:

7.822g $Zn(BF_4)_2$ hydrate (6-7 H_2O, ca 22mmol) are dissolved in 15 ml $CH(OEt)_3$ (90mmol), then the solvent is slowly pumped off (mostly EtOH and $CHO(OEt)_3$) under vacuum near RT. This was repeated three times by adding 8ml $CH(OEt)_3$ (3x48mmol) and pumping off the solvent. The residue becomes increasingly less soluble in added solvent. The final treatment with $CH(OEt)_3$ was left over night and all solvent was pumped off to dryness. In the glove box, the solid was dissolved in 5ml MeCN (ca 100 mmol), stirred for 1 h, solvent pumped off, and the procedure repeated 3 times. Finally the solution was kept for 2 days, decanted from any insoluble precipitate and pumped dry again. The oily residue was washed with hexane and pumped dry several times until a nearly white solid remained. Yield 5.85g. Insufficient EtOH/MeCN exchange may lead to material containing some EtOH. This can be used as well as EtOH is exchanged for the new ligand first.

Synthesis of **1a**. Bz_3TAC (3.20 mmol) was added to a solution of $[(MeCN)_6Ni](BF_4)_2$ (3.20 mmol) in acetonitrile. The dark blue solution was stirred for half an hour. After removing all the volatile materials the crude product was washed three times with ether and dried in vacuo (90% yield). Cooling of a solution in MeCN, saturated at 40 °C, resulted in deep blue crystals. Alternatively, the original reaction solution can be layered with toluene or Et_2O to give crystals of **1a** (same cell constants). Anal. Calcd for $C_{30}H_{36}N_6NiB_2F_8$: C, 50.53; H, 5.09; N, 11.79; Ni, 8.23. Found: C, 50.01; H, 5.44; N, 11.96; Ni, 7.02. Mp 126 °C. UV/Vis (MeCN) ν(nm) / $\varepsilon(cm^{-1}\cdot mol^{-1}\cdot l)$ 945/39, 590/60, 362/93, 292/1261.

1a/Zn, **1b** and **1b/Zn** can be prepared analogously:

100mg of $(oFPhCH2)_3$TAC (0.24mmol) and 95mg of $[Ni(MeCN)_5](BF4)_2$ (0.22 mmol) are dissolved in 1.3 ml MeCN to give a deep blue 0.15 molar solution of **1b** in MeCN (containing 10% free ligand to eliminate excess Ni). Half of the solution is layered with 1 ml of toluene. Blue crystals grow within a day. The excess solution is decanted and the crystals washed with Et_2O to yield 64mg of **1b** (75%).

The other half of the solution is used for NMR. A 0.09 molar solution with no excess ligand was obtained by use of slight excess of $[Ni(MeCN)_5](BF4)_2$ (21.5mg ligand with 26mg or 1.14eq. of $[Ni(MeCN)_5](BF4)_2$ in 0.53 ml of MeCN).

Anal. Calcd for **1b**, $C_{30}H_{33}N_6NiB_2F_{11}$: C, 46.98; H, 4.34; N, 10.96. Found: C, 47.1; H, 4.29; N, 10.9.

99 mg of $(PhCH_2)_3$TAC (0.277 mmol) and 80 mg of $[Zn(MeCN)_4](BF4)_2$ (0.20 mmol) are dissolved in 810 mg MeCN to give a nearly colourless 0.16 molar solution of **1a/Zn** in MeCN (containing 40% excess

$(PhCH_2)_3$TAC). The solution was layered with 1 ml toluene and left standing in the glove box. Colourless crystals grow over night. The solvent was poured off, the residue washed with Et_2O and dried in vacuo.

27.5mg of $(oFPhCH_2)_3$TAC (0.091 mmol) and 42mg of $[Zn(MeCN)_4](BF4)_2$ (0.104 mmol) are dissolved in 0.92 ml MeCN to give a slightly yellowish 0.09 molar solution of **1b/Zn** in MeCN (containing 10% excess $[Zn(MeCN)_4]^{2+}$). Half of the solution is layered with 1 ml of toluene. Colourless crystals grew within a day. The excess solution is decanted and the crystals washed with Et_2O, the other half of the solution is used for NMR.

X-Ray crystallography

Intensity data for **1a, 1b** and **1b/Zn** were collected on a Nonius KappaCCD diffractometer equipped with a low temperature device, using graphite monochromated MoKα radiation (λ= 0.71070 Å). Data were processed using the Nonius Software [1]. Crystal parameters and details on data collection, solution and refinement for the complexes are provided in Table 1. Structure solution, followed by full-matrix least squares refinement was performed using the WinGX-1.70 suite of programs throughout.[2]

Notes on the refinement: in **1b and 1b/Zn** the central NCMe and the two BF_4 groups show a 1:1 disorder. B1 and B1A are refined isotropically. In **1a** one of the phenyl rings of the ligand shows a 1:1 disorder while one of the two BF4 groups show rotational disorder in the ratio 70:30.

1. DENZO-SCALEPACK Z. Otwinowski and W. Minor, " Processing of X-ray Diffraction Data Collected in Oscillation Mode ", Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p.307-326, 1997,C.W. Carter, Jr. & R. M. Sweet, Eds., Academic Press.
2. L.J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838.

Table 1. Crystal and structure refinement data for **1a**, **1b** and **1b/Zn**.

Compound	**1a[BF$_4$]$_2$**	**1b[BF$_4$]$_2$**	**1b/Zn[BF$_4$]$_2$**
Empirical formula	$C_{30}H_{36}B_2F_8N_6Ni$	$C_{30}H_{33}B_2F_{11}N_6Ni$	$C_{30}H_{33}B_2F_{11}N_6Zn$
Formula weight	712.98	766.95	773.61
Temperature	150(2)	250(2)	150(2)
Wavelength / Å	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P -1	P -1
a / Å	10.9500(2)	10.8000(1)	10.7380(2)
b / Å	10.9920(2)	11.7640(1)	11.7460(2)
c / Å	16.3930(4)	14.7490(2)	14.6580(2)
α / °	71.500(1)	105.698(1)	105.6230(6)
β / °	71.165(1)	91.382(1)	91.1820(6)
γ / °	71.625(1)	100.045(1)	100.0630(5)
Volume / Å^3	1720.45(6)	1771.3(3)	1748.62(5)
Z	2	2	2
Density (calculated) / mg/m^3	1.376	1.438	1.469
Absorption coefficient /mm^{-1}	0.637	0.636	0.792
F(000)	736	784	788
Crystal size/ mm	0.45 x 0.38 x 0.15	0.35 x 0.25 x 0.2	0.5 × 0.35× 0.3
Theta range for data collection/ °	3.83 to 29.60	3.34 to 27.54	2.99 to 27.51
Reflections collected	33304	31733	29102
Independent reflections	9592 [R(int) =0.0564]	8097 [R(int) = 0.0285]	7929 [R(int) = 0.0367]
Data/restraints/parameters	9592 / 0 / 518	8097 / 0 / 561	29102 / 0 / 561
Largest diff. peak & hole/ e.Å^{-3}	0.408 and -0.566	0.434 and -0.418	0.529 and -0.699
Final R$^{[a,b]}$ indices [I>2σ(I)]	R_1 = 0.0433 wR_2 = 0.0998	R_1 = 0.0392 wR_2 = 0.1011	R_1 = 0.0405 wR_2 = 0.1000
R$^{[a,b]}$ indices (all data)	R_1 = 0.0695 wR_2 = 0.01107	R_1 = 0.0461 wR_2 = 0.1055	R_1 = 0.0499 wR_2 = 0.1057
Goodness-of-fit on F$^{2[c]}$	1.023	1.029	1.030

[a] $R_1 = \Sigma ||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

[c] $GOF = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)\}^{1/2}$

NMR Spectroscopy

NMR spectra were obtained in acetonitrile with a D_2O capillary for lock and reference. Chemical shifts are reported relative to the acetonitrile solvent signal (1.96ppm for ^{1}H and 1.79ppm for ^{13}C). The ^{1}H chemical shift of neat acetonitrile against HDO (4.70ppm) in the capillary was 2.73ppm and was used to determine the bulk susceptibility shift for the Evans method and to correct the observed ^{19}F shifts. Spectra with excess ligand as internal reference confirmed the validity of this external correction method. NMR spectra were obtained for concentrated solution (0.1M) in MeCN. More dilute solutions give nearly the same chemical shifts and relative line widths at the expense of diminished signal/noise ratios. Diamagnetic reference spectra are obtained from the analogous zinc complexes.
Spectra of the paramagnetic nickel complexes at appropriate repetition times according to the widths of the observed signals (from 40ms acquisition time AQ, 10ms delay D1 for 1500ppm window (SW) for 200,000 scans (NS) for broad ^{13}C signals to 1s (AQ+D1), 40ppm SW and 128 scans for narrow aromatic ^{1}H and ^{13}C signals. T_1 (inversion recovery) and T_2 (Carr-Purcell-Meiboom-Gill, cpmg) measurements were obtained by measuring several windows of 50ppm or less to ensure good 90/180º pulses and 10-30 variable delays for three parameter fits. As T_1 is much shorter than the C-H cross relaxation in most cases, ^{1}H decoupling was found to be unnecessary except for the narrowest ^{13}C signals. T_2 was mostly obtained from the line widths and agreed well with the cpmg measurements done for some peaks.
Assignment of the signals is based on integration, linewidths, ^{2}H NMR signals observed for selectively deuterated **1a** (ring CD_2 at +28 and +9 ppm, benzylic CD_2 at +150ppm and CD_3CN at -30 ppm when measured in CD_3NO_2, details to be included in a future publication), and the reduction of linewidths for broad ^{13}C signals upon selective decoupling of the attached ^{1}H signal. The ring H signals were assigned based on selective NOEs on the two doublets: NOE at ortho CH is 4 times and at benzylic CH_2 2 times larger when irradiated at 4ppm then when irradiated at 3.4ppm (relative to NOE between the two ring signals).
Line widths were determined by Lorentz curve fitting after manual polynomial baseline correction provided by Bruker xwin-nmr, or in the case of broad and isolated peaks by a six-parameter fit for a Lorentz shape curve plus a second order polynomial baseline using ASCII data in ORIGIN (Microcal Origin 6.0). The latter procedure eliminates most of the subjective effects of the manual baseline correction and gave more reliable values. All line shape fits were performed by ORIGIN after conversion of the Bruker NMR spectra to ASCII format.
The measured relaxation times (but not the shifts) are generally increasing upon dilution (about 10% on 4-fold dilution) due to reduced viscosity and outer sphere relaxation due to neighbouring paramagnetic centers. The effect is much larger for diamagnetic signals and the BF_4 anion. The latter indicates increased ion separation on dilution. However, the relative relaxation times within a complex do not change significantly – thus, the data are suitable for structural analysis.
As a diamagnetic reference for the coupling constant in coordinated MeCN commercial $[Pd(MeCN)_4](BF_4)_2$ in CD_3NO_2 gave 139.8 Hz, close to free MeCN (136 Hz).

NMR Data

Table 2. Data are given in the following format and are compared to values obtained from the line shape fit to the full expression for T_1 spin decoupling in red.

Chemical shift in ppm, multiplicity
J=…coupling constant in Hz (suffix F for coupling to F) [J obtain from line shape fit]
(Lorentz) line width W , [W in $^{13}C\{^1H\}$ at region of attached H]
T_2^{-1} as πW ($^{13}C\{^1H\}$), from cpmg [from line shape fit]
T_1^{-1} from inversion recovery [from ^{13}C line shape for ^1H,
or under CH decoupling for ^{13}C]

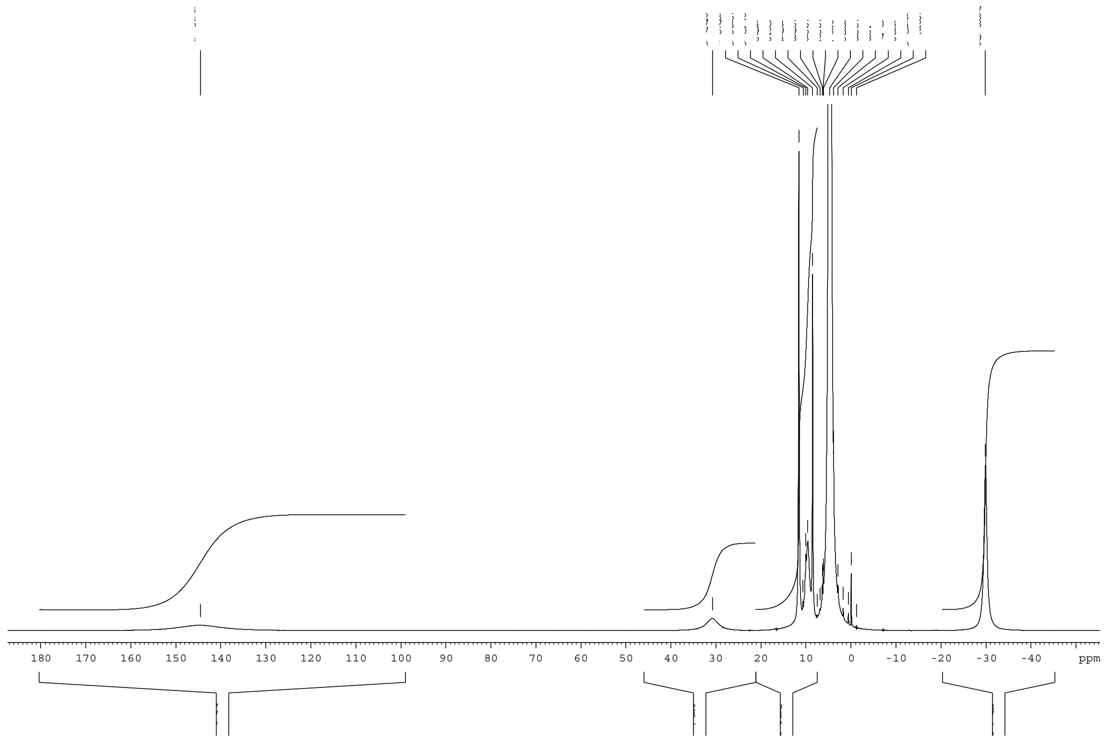
	1a	**1a/Zn**	**1b**	**1b/Zn**
$H_{ax,ring}$	+28.1 1263(3) 3970(10) 3450(230)	3.25d J=9.0	+26 1256(4) 3950(10), 3710(110) 2970(90)	3.36d J=9.0
$H_{eq,ring}$	+9*	4.00d J=9.0	na	4.00d J=9.0
C_{ring}	na	72.7t J=153	na	72.5t J=155
H_{benzl}	+141.8 4604(6) 14460(20) 2750(100)	3.80s 10	+142 4600(10) 14450(40) 2760(70)	3.89s
C_{benzyl}	-88.6 434(5) [396(5)] 1244(16) 534(48)	56.3t J=139	-101 410(10) [389(6)] 1220(20) 444(24)	49.4t J=139 J_F=2.8
$C_{Ph,ipso}$	+441 1191(11) 3740(40) 215(42)	134.0t J=6	+420 1040(30) 3270(90) 174(18)	121.2s J_F=15.4
$H_{Ph,ortho}$	+6.94 357(34) 1120(100) 870(90) [900(60)]	7.4m	7.40 517(8) 1620(30) 1030(220) [1000(80)]	7.37m
$F_{Ph,ortho}$	-	-	-114 282(2) 886(7) 708(1) [724(16)]	-117 J_C=248.9 17(2)
F of BF_4	-151 54.5(1) 171(1) 89.4(2)		-151 53(1) 165(1) 99(1)	-151 2.2(1)

$C_{Ph,ortho}$	138.0 J= - [151(9)] 115(1) [25(1)] 79(4), [79(16)] 59(4) [48(6)]	129.7dd J=7,161	140.0 J= - [156(12)] 95(7) [29(1)] 90(3), 61(6) [91(20)] 56(20) [51(3)] and 162.8d J=”169(2)” [249(3)] “135(3)” -, 53(4) [66(10)] 50(3) [44(4)]	132.5d J=165 and 162.5d J_F=249
$H_{Ph,meta}$	+8.86 53(2) 167(7) 114(12) [130(9)]	7.3m	8.72 66(1) 207(4), 162(3) 109(12) [157(7)] and 8.56 70(1) 220(4) 126(12) [175(6)]	7.23m and 7.17m
$C_{Ph,meta}$	129.0d J=149 [160(1)] “35(1)” [12(2)] 38(7) [38(6)] 18(1) [14.7(2.4)]	131.9td J=6,159	114.5d J=156 [166(1)] “32(10)” [15] -, 23(2) [20(5)] 18(2) [16(2)] And 125.8d J=156, [166(1)] “54(14)” [10] -, 20(2) [9(4)] 18(2) [16(2)]	116.7dd J=168 J_F=24 And 125.8d J=164
$H_{Ph,para}$	+5.80 32(2) 101(7) 61(7) [71(7)]	7.4m	+5.95 33(1) 104(4), 93(2) 67(7) [65(12)]	7.4m
$C_{Ph,para}$	139.5d J=159 [160(1)] “23(1)” [11(1)] 35(4) [35(5)] 12(1) [9.4(1.7)]	129.8td J=7,160	+141.9d J=161 [163(7)] 21(1) [11(1)] 35(4), 19(2) [32(9)] 9(2) [10(1)]	134.5d J=159
H_{MeCN}	-32.6 284(1) 892(1) 327(6)	na	-32.2 271(1) 850(4), 930(60) 330(30)	na
C_{MeCN}	+205 473(3) [337(2)] 1059(7) 77(9)	na	+204 414(5) [314(10)] 986(30), 910(90) 74(7)	na

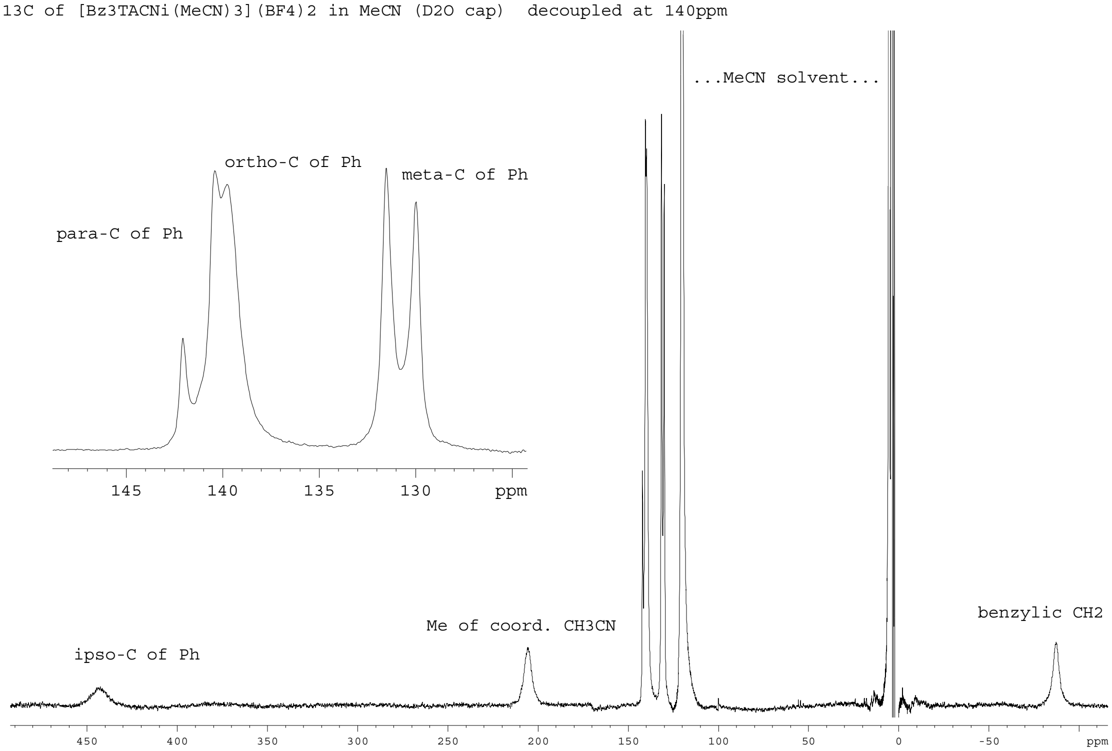
* shift obtained from ^{2}H NMR of the ring deuterated **1** (H_{ax} at 28.8 ppm) (widths 44 for H_{ax} and 91 Hz for H_{eq})

^{1}H (top) and ^{13}C (bottom) NMR spectra of **1a** in MeCN

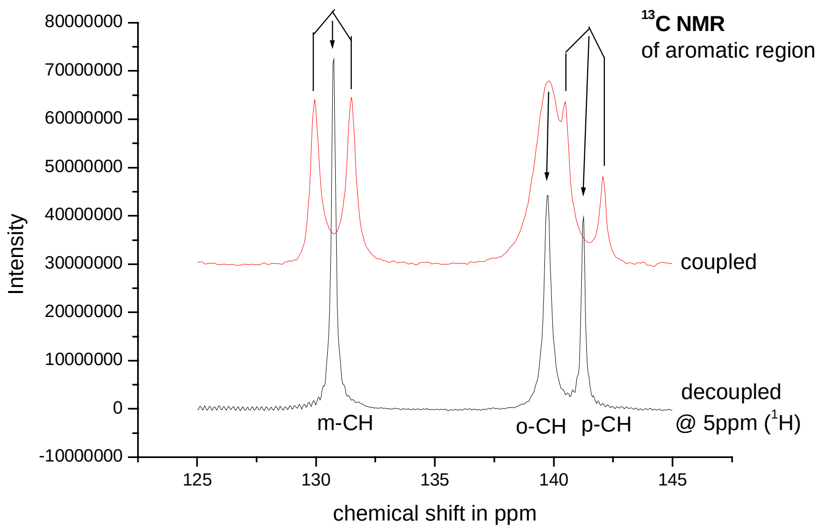
1H NMR of [(PhCH2)3TACNi(MeCN)3] (BF4)2 in MeCN (D2O cap)



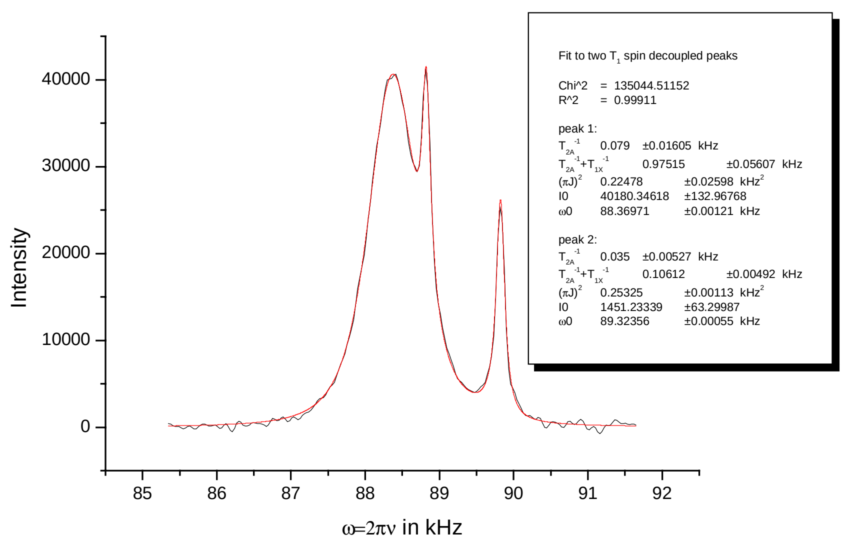
13C of [Bz3TACNi(MeCN)3](BF4)2 in MeCN (D2O cap) decoupled at 140ppm



Comparison of coupled versus decoupled ^{13}C NMR of **1a** in the aromatic region. Note that the ortho-CH signal remains a single peak without {^{1}H} decoupling. It is broadened but not broader the expected J(C-H) coupling as seen for the signals for meta- and para-CH.

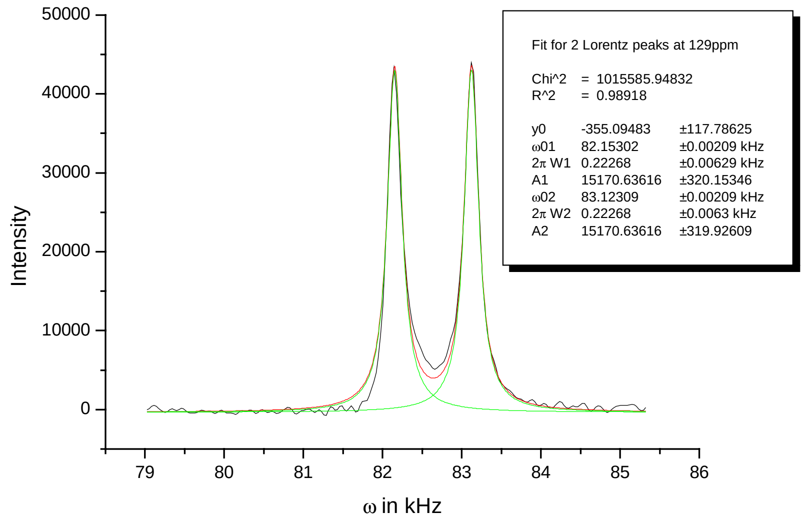


10-Parameter fit with equation eqS1 (5 parameter for each peak) for the ortho- and para-CH signals in **1a**. Minimum T_{2A}^{-1} set to experimental πW of the decoupled spectrum. (Arbitrary intensity units)



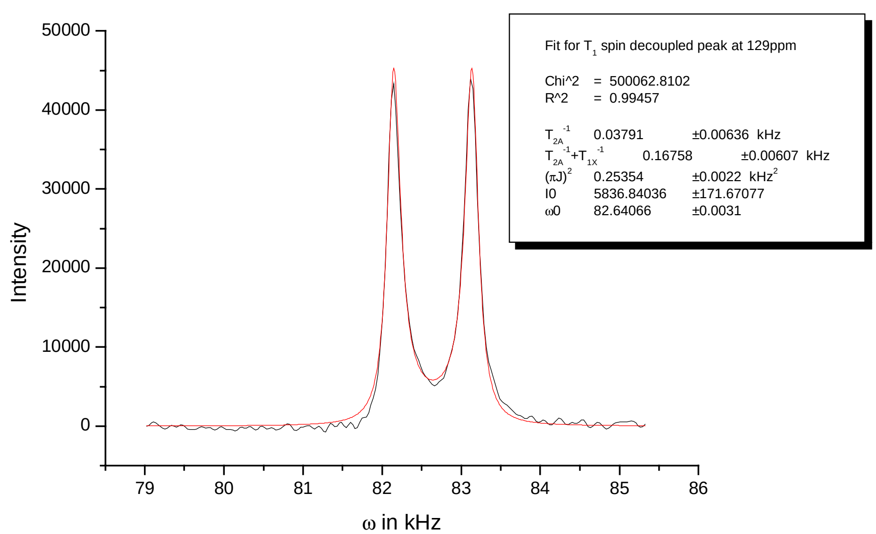
δ=139.77-1.73=138.04ppm, W=25(5)Hz, T_{1X}^{-1}=896(58)Hz, J=151(9)Hz
δ=141.28-1.73=139.55ppm, W=11(2)Hz, T_{1X}^{-1}=71(7)Hz, J=160.2(9) Hz

Coupled ^{13}C NMR signal for the aromatic meta-CH in **1a** with the best fit for two Lorentz-shaped peaks of equal area and width (doublet).



δ=130.71-1.73=128.98ppm, W=35.4(1.0)Hz, „J“=154(2)Hz
The fit is poor in the region between the two peaks.

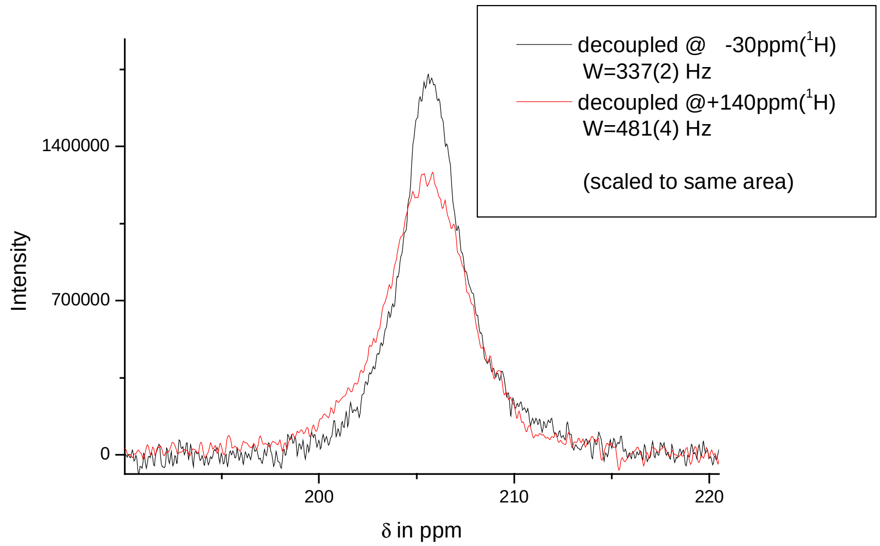
Coupled ^{13}C NMR signal for the aromatic meta-CH in **1a** with the best 5-parameter fit using equation eqS1.

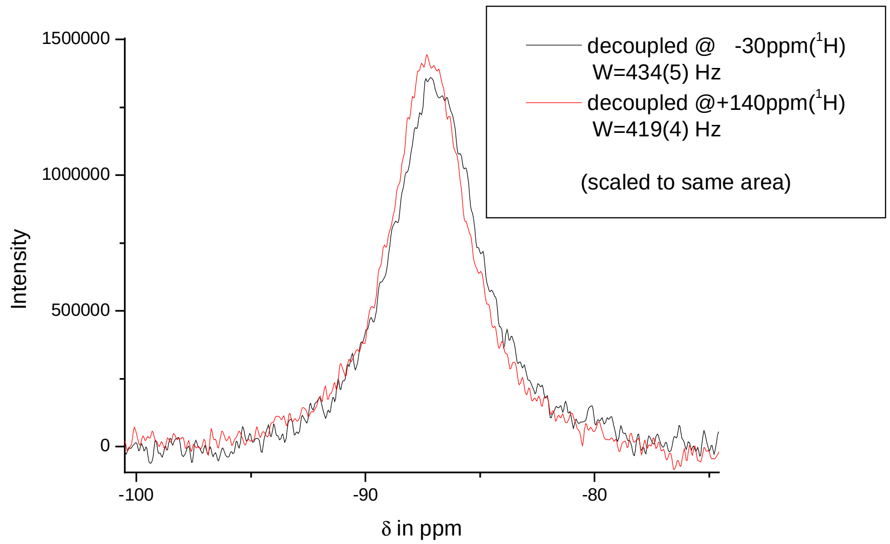


δ=130.71-1.73=128.98ppm, W=12.0(2.0)Hz, T_{1X}^{-1}=130(9)Hz, J=160.3(10)Hz

The fit is much better than for a Lorentz doublet!

Effect of decoupling on ^{13}C NMR peaks much broader than the expected coupling constant: coordinated MeCN (top) and benzylic CH_2 (bottom) in **1a**





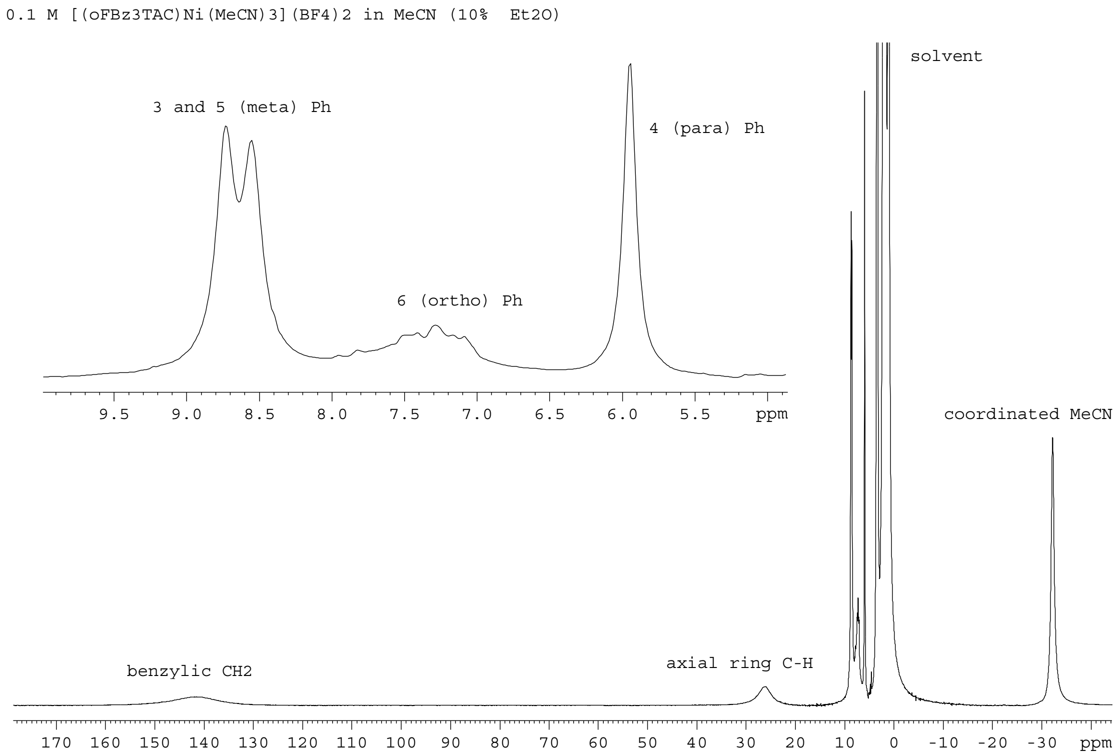
Comparison of the spectra with {^{1}H} decoupling at -30ppm in ^{1}H (black) and at +140ppm (red):

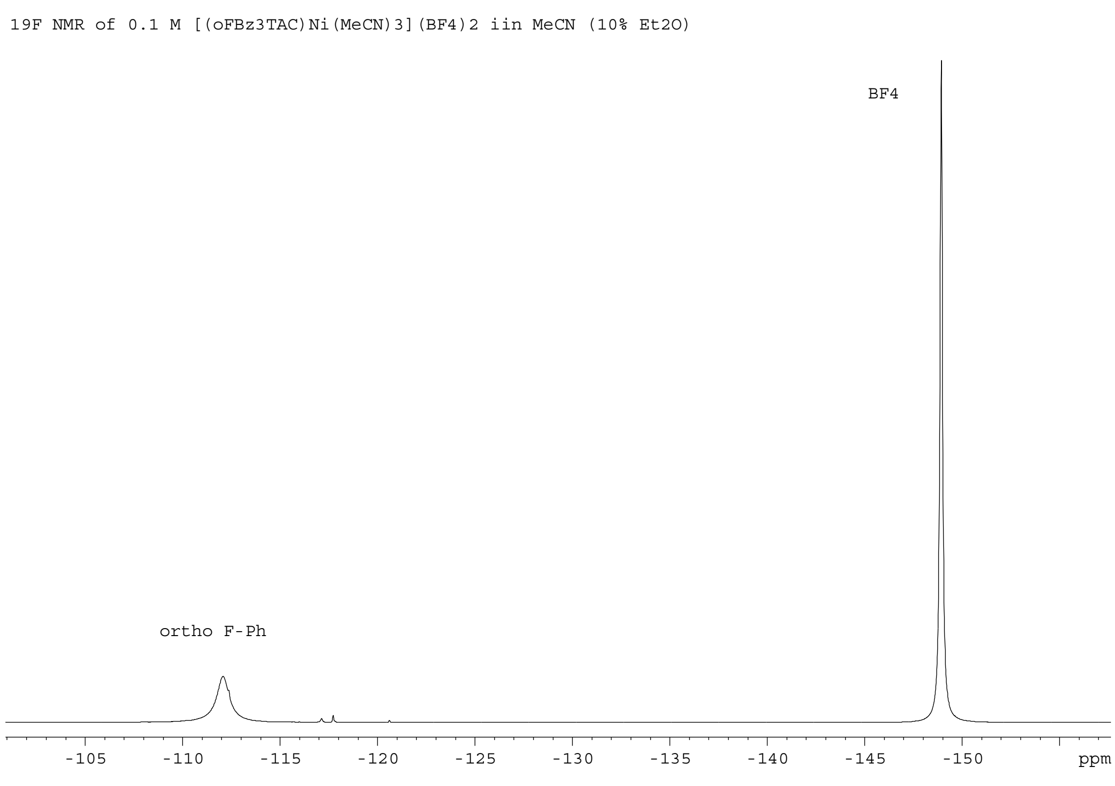
The peak at +205ppm becomes much narrower by decoupling at -30ppm (CH_3CN-Ni)

The peak at -88ppm becomes narrower by decoupling at -140ppm (NCH_2Ph)

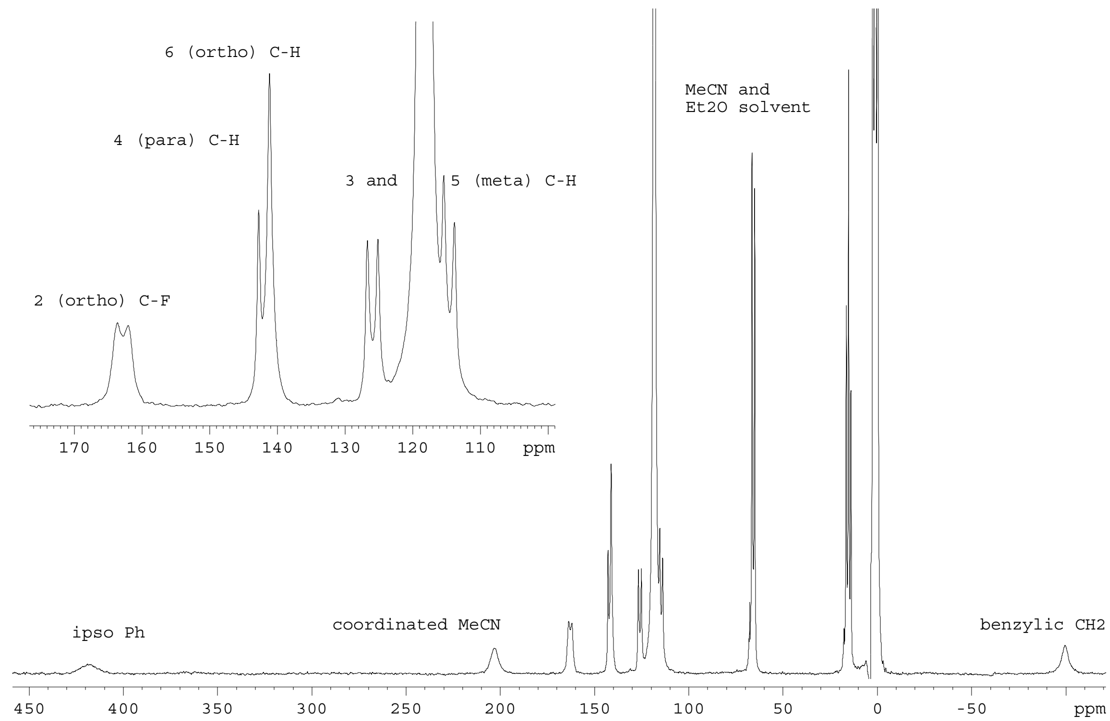
Spectra of **1b** in MeCN (10% Et_2O added as diamagnetic reference)

^{1}H NMR

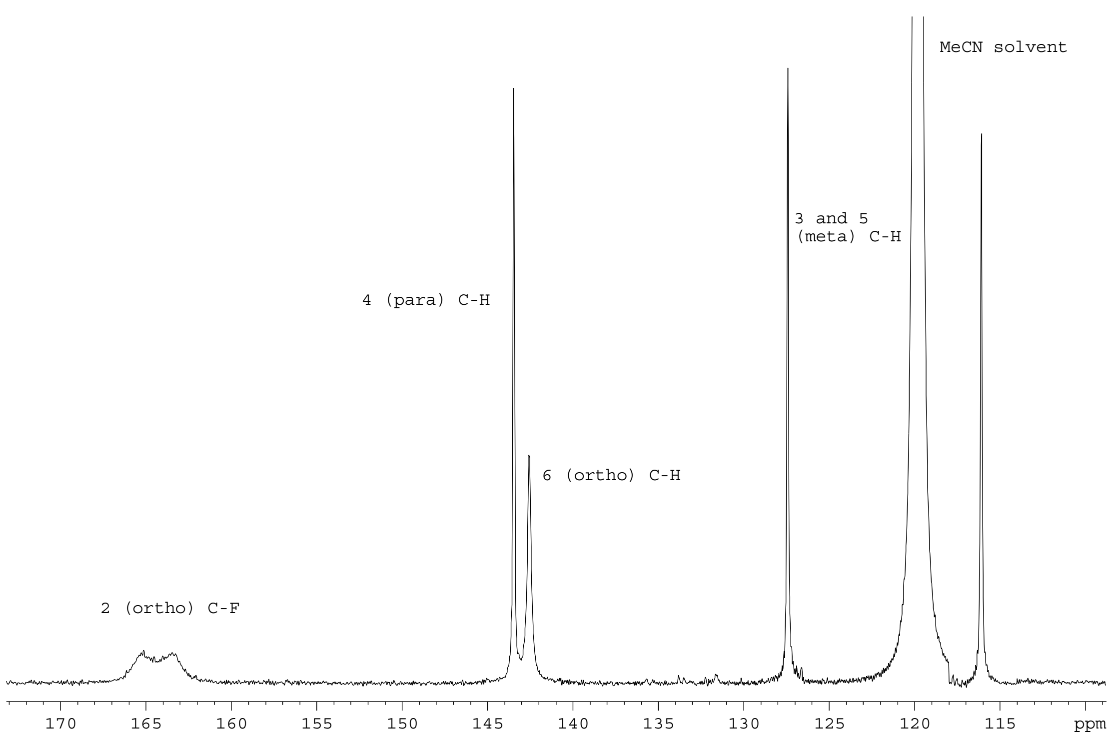




13C {1H at 146ppm} of [(oFBz3TAC)Ni(MeCN)3](BF4)2 in MeCN (10% Et2O)

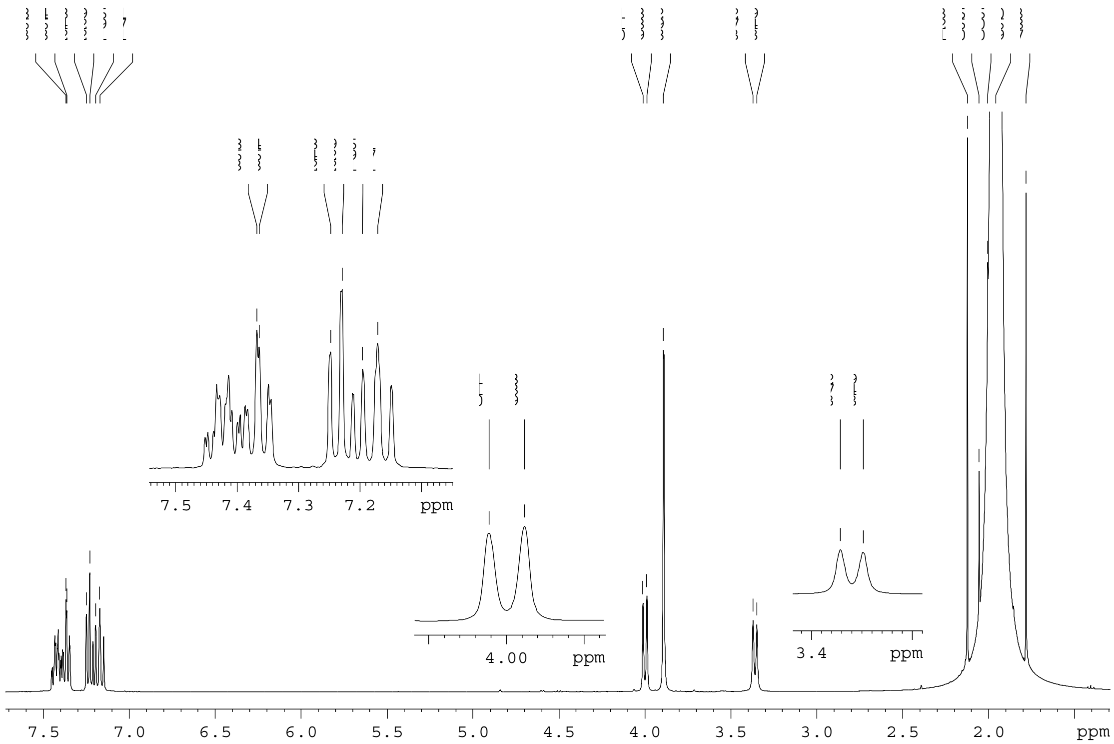


13C {1H at 7ppm} of [(oFBz3TAC)Ni(MeCN)3](BF4)2 in MeCN (10% Et2O)

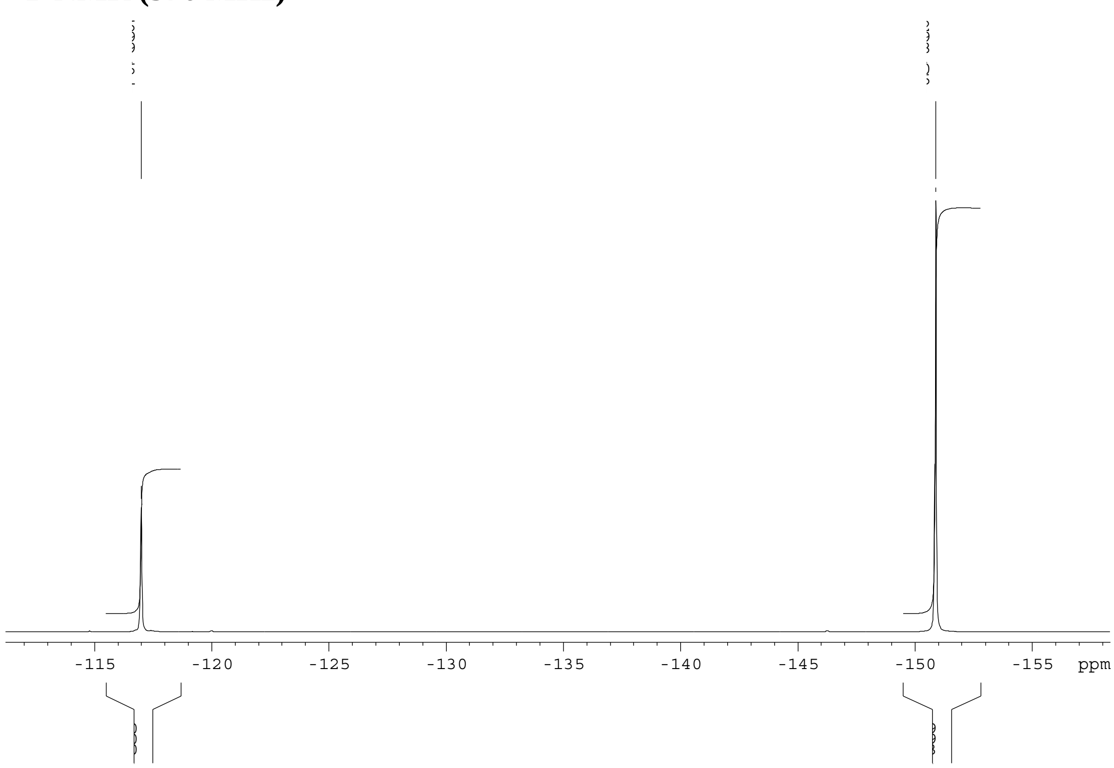


NMR spectra of the Zn analogue of **1b**: **1b/Zn**

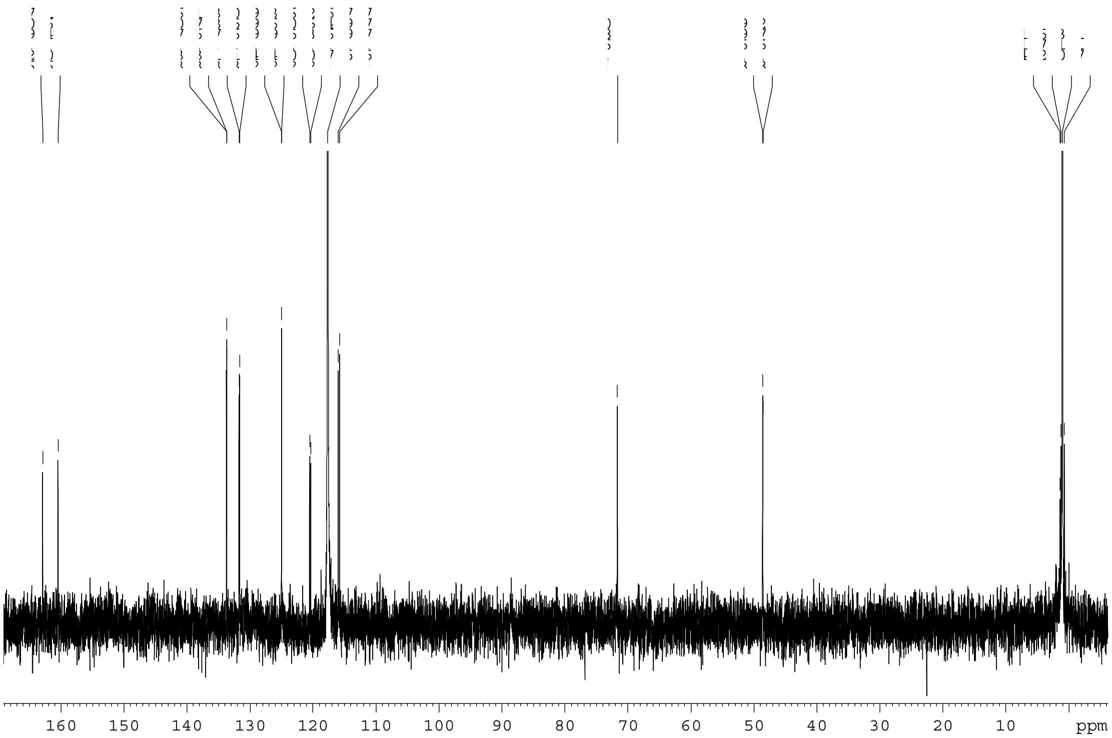
^{1}H NMR (400 MHz)



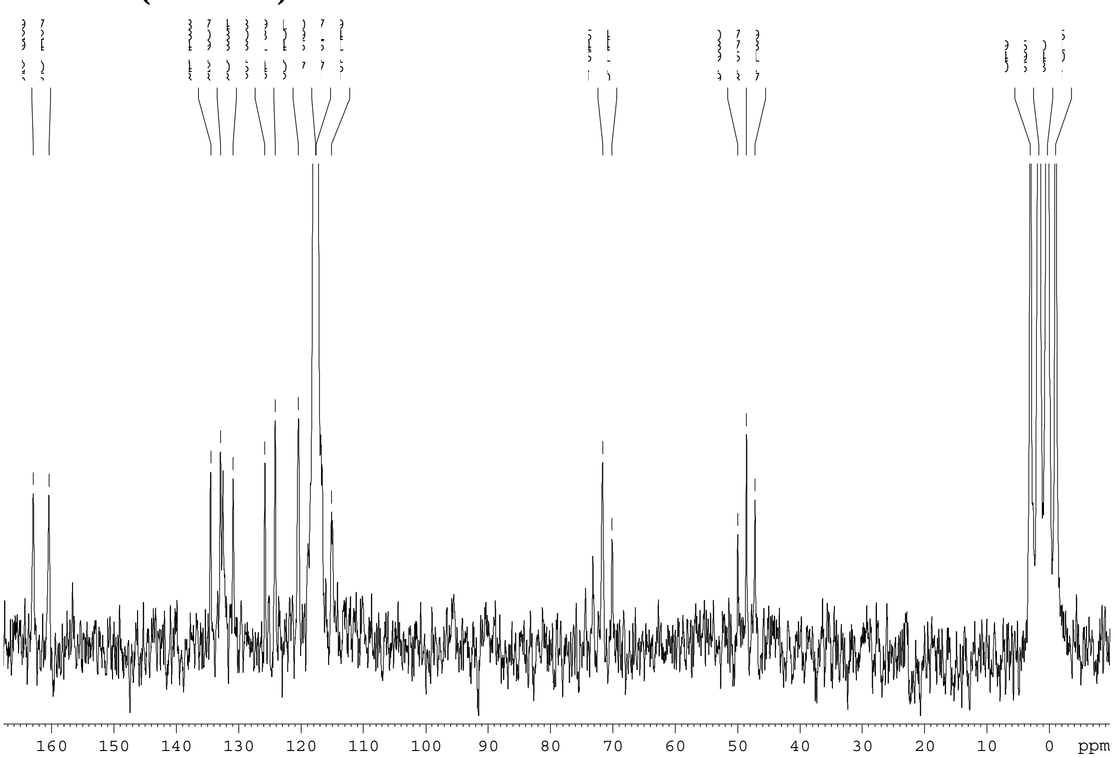
^{19}F NMR (376 MHz)



$^{13}C\{^1H\}$ NMR (100 MHz)

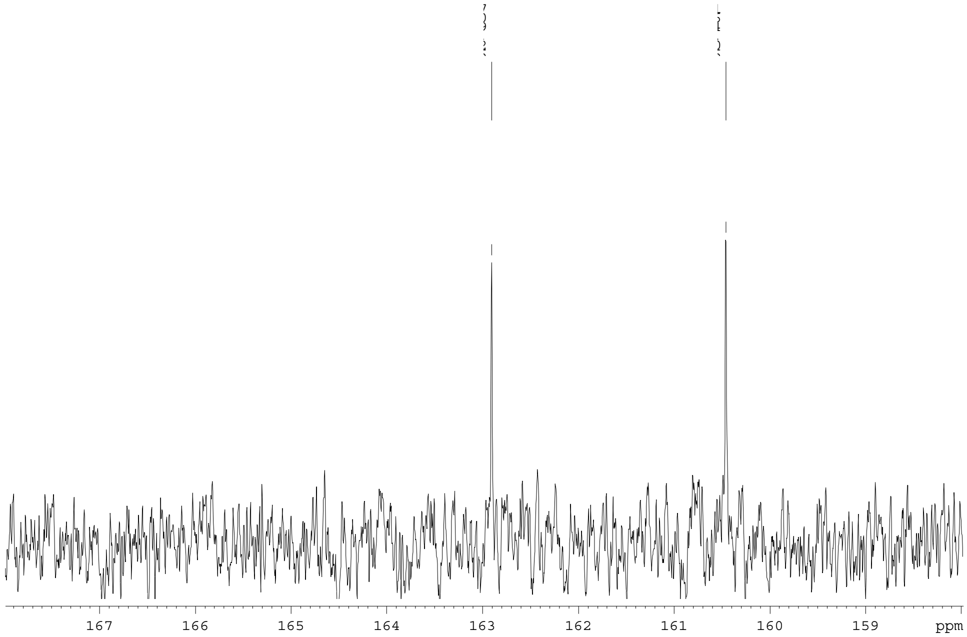


^{13}C NMR (100 MHz)

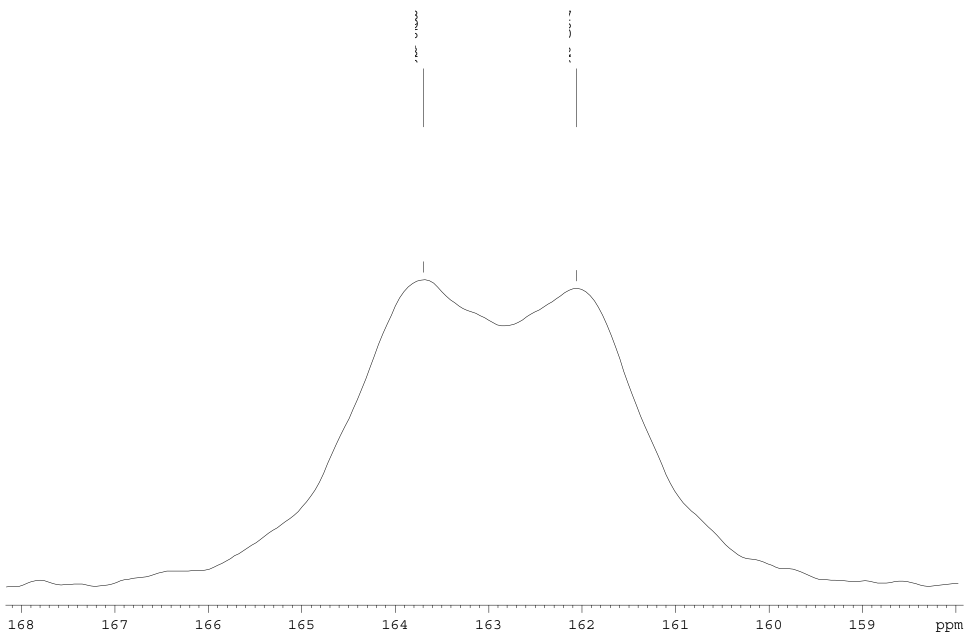


Comparisons of the ^{13}C CF doublets in the zinc and nickel complex:

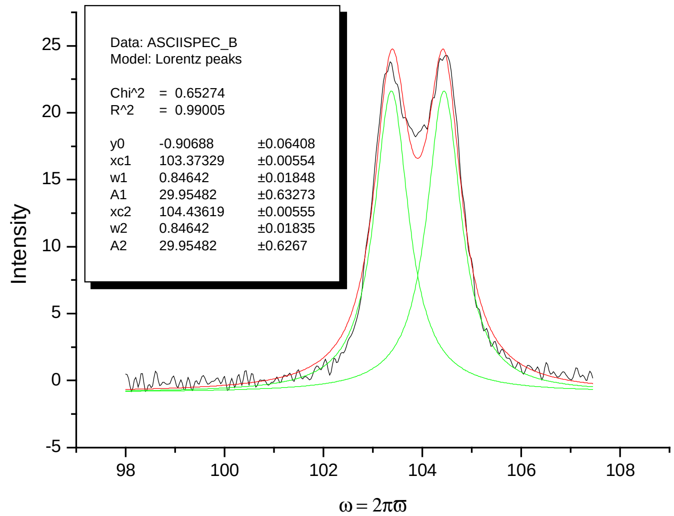
1b/Zn:



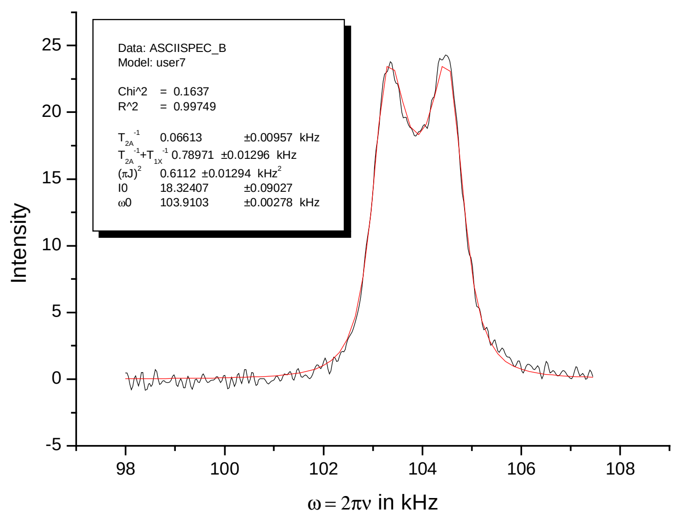
1b:



Fit for the broadened C-F doublet:

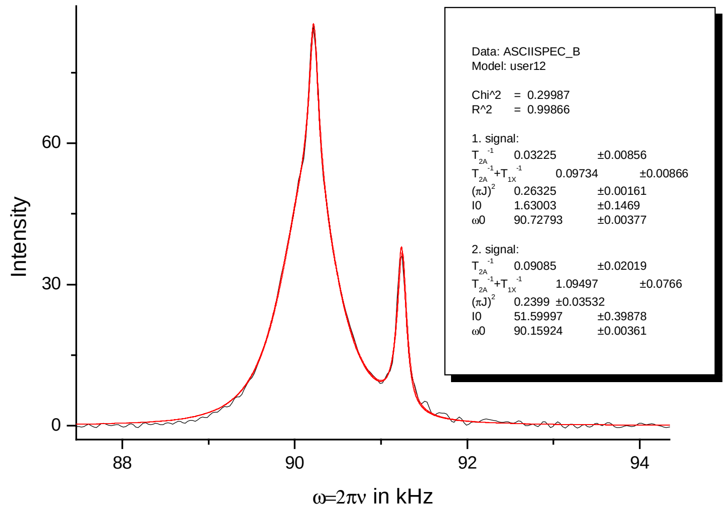


Fit as a Lorentz-shaped doublet is poor. Apparent width is 135(3) Hz with an apparent J=169(2) Hz.



The fit is much better and gives a more reasonable width T_{2A}^{-1}/π=21(3) Hz, T_{1X}^{-1}=724(16) Hz and J=249(3) Hz. These values agree well with the (decoupled) width for the ortho C-H (similar distance) of 29 Hz, the inversion recovery T_{1X}^{-1}=708(1) Hz and J=248.9 Hz in the zinc analog.

Coupled ^{13}C NMR spectrum for the ortho and para-CH signals in **1b** (compare to the same region for **1a** on page S9) with a 10-parameter fit using equation eqS1 for two peaks.



Fit for the o and p-CH:

p-CH: δ=143.5-1.6= 141.9ppm, W=10(3) Hz, J=163(7) Hz, T_{1X}^{-1}=65(12) Hz

o-CH: δ=142.6-1.6= 141.0ppm, W=29(6) Hz, J=156(12) Hz, T_{1X}^{-1}=1004(79) Hz

Derivation of equations

Equations are derived for the Intensity versus x=ω-ω_0 based on ref 3, J in Hz is used (rather than in radian). The real part of the complex expression obtained by the matrix product $\mathbf{WA^{-1}1}$ has to be derived. As many terms are involved, the procedure is done in many small steps to aid understanding. This leads to full expressions for the line shape for the doublet (2x2 matrix), triplet (3x3) and quartet (4x4) case as eqS1 (page S17), eqS3 (S23) and eqS4 (S30), respectively.
More user friendly approximate solutions for coalesced signals are derived by Taylor expansion around x=0. This over-estimates the apparent line width but gives the appropriate functional forms. This form is corrected empirically, by a best fit procedure as described and validated in detail on page S34.

Doublet Case:

$$A = \begin{bmatrix} ix + \pi Ji - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1} & \tfrac{1}{2}T_{1X}^{-1} \\ \tfrac{1}{2}T_{1X}^{-1} & ix - \pi Ji - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1} \end{bmatrix}$$

$$x = 2\pi(\nu - \nu_0)$$

$$|A| = \left(ix - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1}\right)^2 + \pi^2 J^2 - \tfrac{1}{4}T_{1X}^{-2}$$

$$A^{-1} = \begin{bmatrix} ix - \pi Ji - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1} & -\tfrac{1}{2}T_{1X}^{-1} \\ -\tfrac{1}{2}T_{1X}^{-1} & ix + \pi Ji - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1} \end{bmatrix} / |A|$$

$$I(x) = \mathrm{Re}\{W \bullet A^{-1} \bullet 1\}$$

$$W \bullet A^{-1} \bullet 1 = \begin{pmatrix}1\\1\end{pmatrix} \bullet A^{-1} \bullet \begin{pmatrix}1\\1\end{pmatrix} = 2\frac{ix - T_{2A}^{-1} - T_{1X}^{-1}}{\left(ix - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1}\right)^2 + \pi^2 J^2 - \tfrac{1}{4}T_{1X}^{-2}} =$$

$$= 2\frac{ix - T_{2A}^{-1} - T_{1X}^{-1}}{-x^2 - ix\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2} =$$

$$= 2\frac{\left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)\left(-x^2 + ix\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)}{\left(-x^2 - ix\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)\left(-x^2 + ix\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)} =$$

$$= 2\frac{i\,\mathrm{Im} + \left(T_{2A}^{-1} + T_{1X}^{-1}\right)\left(x^2 - T_{2A}^{-2} - T_{2A}^{-1}T_{1X}^{-1} - \pi^2 J^2\right) - \left(2T_{2A}^{-1} + T_{1X}^{-1}\right)x^2}{\left(-x^2 + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)^2 + x^2\left(2T_{2A}^{-1} + T_{1X}^{-1}\right)^2} =$$

$$= 2\frac{i\,\mathrm{Im} - \left(T_{2A}^{-1} + T_{1X}^{-1}\right)\left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right) - T_{2A}^{-1}x^2}{x^4 + x^2\left(\left(2T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - 2T_{2A}^{-2} - 2T_{2A}^{-1}T_{1X}^{-1} - 2\pi^2 J^2\right) + \left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)^2} =$$

$$= 2\frac{i\,\mathrm{Im} - \left(T_{2A}^{-1} + T_{1X}^{-1}\right)\left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right) - T_{2A}^{-1}x^2}{x^4 + x^2\left(2T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} - 2\pi^2 J^2\right) + \left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)^2}$$

With I(x=0) = I_0 = $\dfrac{-2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)}{\left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)}$

$$I(x) = I_0 \frac{\left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)\frac{T_{2A}^{-1}}{T_{2A}^{-1}+T_{1X}^{-1}} x^2 + \left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)^2}{x^4 + x^2\left(2T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} - 2\pi^2 J^2\right) + \left(T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2\right)^2}$$

with

$$x = \omega - \omega_0$$

$$P1 = T_{2A}^{-1}; P2 = T_{2A}^{-1} + T_{1X}^{-1}; P3 = \pi^2 J^2; P4 = I_0; P5 = \omega_0$$

$$I(x) = P4 \frac{\left(P1P2 + P3\right)\frac{P1}{P2}(\omega - P5)^2 + \left(P1P2 + P3\right)^2}{(\omega - P5)^4 + (\omega - P5)^2\left(P1^2 + P2^2 - 2P3\right) + \left(P1P2 + P3\right)^2} \left(eqS1\right)$$

The latter equation (eqS1) is used as user defined equation for 5 parameter fitting in ORIGIN (or 10 parameter fitting for two peaks)

Conditions for coalescence to a single peak:

$$I(x)=I_0\frac{\left(T_{2A}^{-2}+T_{2A}^{-1}T_{1X}^{-1}+\pi^2J^2\right)\frac{T_{2A}^{-1}}{T_{2A}^{-1}+T_{1X}^{-1}}x^2+\left(T_{2A}^{-2}+T_{2A}^{-1}T_{1X}^{-1}+\pi^2J^2\right)^2}{x^4+x^2\left(2T_{2A}^{-2}+2T_{2A}^{-1}T_{1X}^{-1}+T_{1X}^{-2}-2\pi^2J^2\right)+\left(T_{2A}^{-2}+T_{2A}^{-1}T_{1X}^{-1}+\pi^2J^2\right)^2}=I_0\frac{Ax^2+B}{x^4+Cx^2+B}$$

$$I'(x)=I_0\frac{2Ax(x^4+Cx^2+B)-(4x^3+2Cx)(Ax^2+B)}{(x^4+Cx^2+B)^2}=$$

$$=I_0\frac{2Ax^5+2ACx^3+2ABx-4Ax^5-2ACx^3-4Bx^3-2BCx}{(x^4+Cx^2+B)^2}=$$

$$=I_0\frac{-2Ax^5-4Bx^3+2(A-C)Bx}{(x^4+Cx^2+B)^2}$$

$coalescence:$

$$I''(x=0)=I_0\frac{2(A-C)B^2}{B^3}=0\Rightarrow A=C$$

$$\left(T_{2A}^{-2}+T_{2A}^{-1}T_{1X}^{-1}+\pi^2J^2\right)\frac{T_{2A}^{-1}}{T_{2A}^{-1}+T_{1X}^{-1}}=2T_{2A}^{-2}+2T_{2A}^{-1}T_{1X}^{-1}+T_{1X}^{-2}-2\pi^2J^2$$

$$T_{2A}^{-3}+T_{2A}^{-2}T_{1X}^{-1}+T_{2A}^{-1}\pi^2J^2=2T_{2A}^{-3}+2T_{2A}^{-2}T_{1X}^{-1}+T_{2A}^{-1}T_{1X}^{-2}-2T_{2A}^{-1}\pi^2J^2+2T_{1X}^{-1}T_{2A}^{-2}+2T_{2A}^{-1}T_{1X}^{-2}+T_{1X}^{-3}-2T_{1X}^{-1}\pi^2J^2$$

$$(3T_{2A}^{-1}+2T_{1X}^{-1})\pi^2J^2=T_{2A}^{-3}+3T_{2A}^{-2}T_{1X}^{-1}+3T_{2A}^{-1}T_{1X}^{-2}+T_{1X}^{-3}=(T_{1X}^{-1}+T_{2A}^{-1})^3$$

$$\pi^2J^2=\frac{(T_{1X}^{-1}+T_{2A}^{-1})^3}{3T_{2A}^{-1}+2T_{1X}^{-1}}(eq.3)$$

Approximate solution for the maxima at x=+/-πΔ (Δ apparent J) before coalescence:

$$I'(\pi\Delta) = I_0 \frac{-2A(\pi\Delta)^5 - 4B(\pi\Delta)^3 + 2(A-C)B(\pi\Delta)}{((\pi\Delta)^4 + C(\pi\Delta)^2 + B)^2} = 0$$

$$\Rightarrow -2A(\pi\Delta)^4 - 4B(\pi\Delta)^2 + 2(A-C)B = 0$$

$$(\pi\Delta)^4 + 2\tfrac{B}{A}(\pi\Delta)^2 - (A-C)\tfrac{B}{A} = 0$$

$$(\pi\Delta)^2 = -\tfrac{B}{A} + \sqrt{(\tfrac{B}{A})^2 + B + C\tfrac{B}{A}} = -(T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} + \pi^2 J^2 + \pi^2 J^2 \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})$$

$$+\sqrt{\begin{matrix}(T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} + \pi^2 J^2 + \pi^2 J^2 \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})^2 + (T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2)^2 \\ -(2T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} - 2\pi^2 J^2)(T_{2A}^{-2} + 2T_{2A}^{-1}T_{1X}^{-1} + T_{1X}^{-2} + \pi^2 J^2 + \pi^2 J^2 \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\end{matrix}} =$$

$$= -(T_{2A}^{-1} + T_{1X}^{-1})^2 - (1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2$$

$$+\sqrt{\begin{matrix}(T_{2A}^{-1} + T_{1X}^{-1})^4 + 2(T_{2A}^{-1} + T_{1X}^{-1})^2(1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2 + (1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})^2 \pi^4 J^4 + T_{2A}^{-2}(T_{2A}^{-1} + T_{1X}^{-1})^2 \\ + 2T_{2A}^{-1}(T_{2A}^{-1} + T_{1X}^{-1})\pi^2 J^2 + \pi^4 J^4 - T_{2A}^{-2}(T_{2A}^{-1} + T_{1X}^{-1})^2 - T_{2A}^{-2}(1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2 - (T_{2A}^{-1} + T_{1X}^{-1})^4 \\ -(T_{2A}^{-1} + T_{1X}^{-1})^2(1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2 + 2(T_{2A}^{-1} + T_{1X}^{-1})^2 \pi^2 J^2 + 2(1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^4 J^4\end{matrix}} =$$

$$= -(T_{2A}^{-1} + T_{1X}^{-1})^2 - (1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2$$

$$+\sqrt{\begin{matrix}(4 + 4\tfrac{T_{1X}^{-1}}{T_{2A}^{-1}} + \tfrac{T_{1X}^{-2}}{T_{2A}^{-2}})\pi^4 J^4 \\ + (4T_{2A}^{-2} + 8T_{1X}^{-1}T_{2A}^{-1} + 3T_{1X}^{-2})\pi^2 J^2 + (2T_{1X}^{-1}T_{2A}^{-1} + T_{1X}^{-2})\tfrac{T_{1X}^{-1}}{T_{2A}^{-1}}\pi^2 J^2\end{matrix}} =$$

$$= -(T_{2A}^{-1} + T_{1X}^{-1})^2 - (1 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})\pi^2 J^2$$

$$+\sqrt{(4T_{2A}^{-2} + 8T_{1X}^{-1}T_{2A}^{-1} + 5T_{1X}^{-2} + \tfrac{T_{1X}^{-3}}{T_{2A}^{-1}})\pi^2 J^2 + (2 + \tfrac{T_{1X}^{-1}}{T_{2A}^{-1}})^2 \pi^4 J^4} =$$

$$= T_{2A}[-T_{2A}^{-1}(T_{2A}^{-1} + T_{1X}^{-1})^2 - (T_{2A}^{-1} + T_{1X}^{-1})\pi^2 J^2 +$$

$$\sqrt{(4T_{2A}^{-4} + 8T_{1X}^{-1}T_{2A}^{-3} + 5T_{1X}^{-2}T_{2A}^{-2} + T_{1X}^{-3}T_{2A}^{-1})\pi^2 J^2 + (2T_{2A}^{-1} + T_{1X}^{-1})^2 \pi^4 J^4}]$$

Expansion in T_{2A}^{-1}(<<T_{1X}^{-1}, πJ) to second order:

$$(\pi\Delta)^2 = T_{2A}[-T_{1X}^{-1}\pi^2 J^2 + \sqrt{T_{1X}^{-2}\pi^4 J^4}]$$

$$-T_{1X}^{-2} - \pi^2 J^2 + [T_{1X}^{-3}\pi^2 J^2 + 4T_{1X}^{-1}\pi^4 J^4]/2\sqrt{T_{1X}^{-2}\pi^4 J^4}$$

$$-\tfrac{1}{2}T_{2A}^{-1}T_{1X}^{-1} - \frac{T_{2A}^{-1}T_{1X}^{-3}}{8\pi^2 J^2} = -T_{1X}^{-2} - \pi^2 J^2 + \tfrac{1}{2}T_{1X}^{-2} + 2\pi^2 J^2 - \tfrac{1}{2}T_{2A}^{-1}T_{1X}^{-1} - \frac{T_{2A}^{-1}T_{1X}^{-3}}{8\pi^2 J^2} =$$

$$= \pi^2 J^2 - \tfrac{1}{2}T_{1X}^{-2} - \tfrac{1}{2}T_{2A}^{-1}T_{1X}^{-1} - \frac{T_{2A}^{-1}T_{1X}^{-3}}{8\pi^2 J^2}$$

$$\approx \pi^2 J^2 - \tfrac{1}{2}T_{1X}^{-2}$$

Approximate solutions for the line widths of the coalesced peak:

- for singlets: Taylor expansion of $1/\{WA^{-1}1\}$ in (ix) gives:

$$f(ix) = 2/(W \bullet A^{-1} \bullet 1) = \frac{\left(ix - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1}\right)^2 + \pi^2 J^2 - \tfrac{1}{4}T_{1X}^{-2}}{ix - T_{2A}^{-1} - T_{1X}^{-1}}$$

$$f(0) = \frac{\left(T_{2A}^{-1} + \tfrac{1}{2}T_{1X}^{-1}\right)^2 + \pi^2 J^2 - \tfrac{1}{4}T_{1X}^{-2}}{T_{2A}^{-1} + T_{1X}^{-1}} = T_{2A}^{-1} + \frac{\pi^2 J^2}{T_{2A}^{-1} + T_{1X}^{-1}}$$

$$f'(ix) = \frac{2\left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)\left(ix - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1}\right) - \left(ix - T_{2A}^{-1} - \tfrac{1}{2}T_{1X}^{-1}\right)^2 - \pi^2 J^2 + \tfrac{1}{4}T_{1X}^{-2}}{\left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)^2} =$$

$$= \frac{2(ix)^2 - 2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)(ix) + 2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)\left(T_{2A}^{-1} + \tfrac{1}{2}T_{1X}^{-1}\right) - \left(T_{2A}^{-1} + \tfrac{1}{2}T_{1X}^{-1}\right)^2 - \pi^2 J^2 + \tfrac{1}{4}T_{1X}^{-2}}{\left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)^2} =$$

$$= \frac{2(ix)^2 - 2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)(ix) + \left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - \pi^2 J^2}{\left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)^2}$$

$$\Rightarrow f'(0) = \frac{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - \pi^2 J^2}{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2}$$

$\Rightarrow$

$$f(ix) \approx T_{2A}^{-1} + \frac{\pi^2 J^2}{T_{2A}^{-1} + T_{1X}^{-1}} + \frac{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - \pi^2 J^2}{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2}(ix) =$$

$$= \frac{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - \pi^2 J^2}{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2}\left(\underbrace{\frac{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 T_{2A}^{-1} + \left(T_{2A}^{-1} + T_{1X}^{-1}\right)\pi^2 J^2}{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2 - \pi^2 J^2}}_{\pi W} + (ix)\right)$$

Taylor expansion in $\pi^2 J^2$:

$$\Rightarrow \pi W \approx T_{2A}^{-1} + \frac{T_{1X}^{-1} + 2T_{2A}^{-1}}{\left(T_{2A}^{-1} + T_{1X}^{-1}\right)^2}\pi^2 J^2 \quad \text{(eq.S2)}$$

This approximation constructs an approximate Lorentz peak around x=0. The true line shape is “flattened” at this point, thus (eq. S2) over-estimates the widths compared to the least-square Lorentz fit.

Taylor expansion around y=1/x=0 (infinite x):

$$I(x) = C\frac{ix - T_{2A}^{-1} - T_{1X}^{-1}}{-x^2 - ix\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-2} + T_{2A}^{-1}T_{1X}^{-1} + \pi^2 J^2} =$$

$$= C\frac{iy - (T_{2A}^{-1} + T_{1X}^{-1})y^2}{-1 - iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + \ldots}$$

$$I(y=0) = 0$$

$$I'(y) = C\frac{(-1 - iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right))(i - 2(T_{2A}^{-1} + T_{1X}^{-1})y) + iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right)(i - (T_{2A}^{-1} + T_{1X}^{-1})y) + \ldots}{(-1 - iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + \ldots)^2} =$$

$$= C\frac{-i + y(2T_{2A}^{-1} + 2T_{1X}^{-1}) + \ldots}{1 + 2iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + \ldots}$$

$$I'(y=0) = -Ci$$

$$I''(y) = C\frac{(1 + 2iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right))(2T_{2A}^{-1} + 2T_{1X}^{-1}) - 2i\left(2T_{2A}^{-1} + T_{1X}^{-1}\right)(-i + y(2T_{2A}^{-1} + 2T_{1X}^{-1})) + \ldots}{(1 + 2iy\left(2T_{2A}^{-1} + T_{1X}^{-1}\right) + \ldots)^2}$$

$$I''(y=0) = C\frac{2T_{2A}^{-1} + 2T_{1X}^{-1} - 2\left(2T_{2A}^{-1} + T_{1X}^{-1}\right)}{1} = -2CT_{2A}^{-1}$$

$$I(y) \approx -C(iy + T_{2A}^{-1}y^2)$$

and

$$\left|\mathrm{Re}(I(y))\right| \approx CT_{2A}^{-1}y^2 = C\frac{T_{2A}^{-1}}{x^2}$$

Expansion of a Lorentz function with width W around y=1/x=0:

$$I(x) = \frac{C}{ix + \pi W} = C\frac{y}{i + \pi W y}$$

$$I(y=0) = 0$$

$$I'(y) = C\frac{(i + \pi W y)1 - \pi W y}{(i + \pi W y)^2} = C\frac{i}{-1 + 2\pi W y i + \ldots}$$

$$I'(y=0) = -Ci$$

$$I''(y) = C\frac{(-1 + 2\pi W y i)0 + 2\pi W + \ldots}{(-1 + 2\pi W y i + \ldots)^2} = C\frac{2\pi W + \ldots}{1 - 4\pi W y i + \ldots}$$

$$I''(y=0) = 2\pi W C$$

$$I(y) \approx -Ciy + \pi W C y^2$$

and

$$\mathrm{Re}(I(y)) \approx \pi W C y^2 = C\frac{\pi W}{x^2}$$

Therefore:

$$\pi W \approx T_{2A}^{-1}$$

This approximation under-estimates the width for a least-square Lorentz fit.

<u>Triplet Case:</u>

$$A = \begin{bmatrix} ix + 2\pi Ji - T_{2A}^{-1} - T_{1X}^{-1} & T_{1X}^{-1} & 0 \\ \frac{1}{2}T_{1X}^{-1} & ix - T_{2A}^{-1} - T_{1X}^{-1} & \frac{1}{2}T_{1X}^{-1} \\ 0 & T_{1X}^{-1} & ix - 2\pi Ji - T_{2A}^{-1} - T_{1X}^{-1} \end{bmatrix}$$

$$x = 2\pi(\nu - \nu_0)$$

$$|A| = \left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)^3 + 4\pi^2 J^2 \left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right) - \left(ix - T_{2A}^{-1} - T_{1X}^{-1}\right)T_{1X}^{-2} =$$

$$= (ix)^3 - 3(T_{2A}^{-1} + T_{1X}^{-1})(ix)^2 + (3(T_{2A}^{-1} + T_{1X}^{-1})^2 + 4\pi^2 J^2 - T_{1X}^{-2})(ix) - (T_{2A}^{-1} + T_{1X}^{-1})^3$$

$$- 4\pi^2 J^2 \left(T_{2A}^{-1} + T_{1X}^{-1}\right) + T_{2A}^{-1}T_{1X}^{-2} - T_{1X}^{-3} =$$

$$= (ix)^3 - 3(T_{2A}^{-1} + T_{1X}^{-1})(ix)^2 + (3T_{2A}^{-2} + 6T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 4\pi^2 J^2)(ix)$$

$$- T_{2A}^{-3} - 3T_{2A}^{-2}T_{1X}^{-1} - 2T_{2A}^{-1}T_{1X}^{-2} - 4\pi^2 J^2 \left(T_{2A}^{-1} + T_{1X}^{-1}\right)$$

$$A^{-1} =$$

$$= \frac{\begin{bmatrix} (ix - T_{2A}^{-1} - T_{1X}^{-1})^2 - 2\pi Ji(ix - T_{2A}^{-1} - T_{1X}^{-1}) - \frac{1}{2}T_{1X}^{-2} & -T_{1X}^{-1}(ix - T_{2A}^{-1} - T_{1X}^{-1} - 2\pi Ji) & \frac{1}{2}T_{1X}^{-2} \\ -\frac{1}{2}T_{1X}^{-1}(ix - T_{2A}^{-1} - T_{1X}^{-1} - 2\pi Ji) & (ix - T_{2A}^{-1} - T_{1X}^{-1})^2 + 4\pi^2 J^2 & -\frac{1}{2}T_{1X}^{-1}(ix - T_{2A}^{-1} - T_{1X}^{-1} + 2\pi Ji) \\ \frac{1}{2}T_{1X}^{-2} & -T_{1X}^{-1}(ix - T_{2A}^{-1} - T_{1X}^{-1} + 2\pi Ji) & (ix - T_{2A}^{-1} - T_{1X}^{-1})^2 + 2\pi Ji(ix - T_{2A}^{-1} - T_{1X}^{-1}) - \frac{1}{2}T_{1X}^{-2} \end{bmatrix}}{|A|}$$

$$I(x) = \mathrm{Re}\{W \bullet A^{-1} \bullet 1\}$$

$$W \bullet A^{-1} \bullet 1 = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} \bullet A^{-1} \bullet \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} =$$

$$= \frac{4(ix - T_{2A}^{-1} - T_{1X}^{-1})^2 - 4T_{1X}^{-1}(ix - T_{2A}^{-1} - T_{1X}^{-1}) + 8\pi^2 J^2}{(ix)^3 - 3(T_{2A}^{-1} + T_{1X}^{-1})(ix)^2 + (3T_{2A}^{-2} + 6T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 4\pi^2 J^2)(ix) - T_{2A}^{-3} - 3T_{2A}^{-2}T_{1X}^{-1} - 2T_{2A}^{-1}T_{1X}^{-2} - 4\pi^2 J^2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)} =$$

$$= 4\frac{(ix)^2 - (ix)(2T_{2A}^{-1} + 3T_{1X}^{-1}) + T_{2A}^{-2} + 3T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 2\pi^2 J^2}{(ix)^3 - 3(T_{2A}^{-1} + T_{1X}^{-1})(ix)^2 + (3T_{2A}^{-2} + 6T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 4\pi^2 J^2)(ix) - T_{2A}^{-3} - 3T_{2A}^{-2}T_{1X}^{-1} - 2T_{2A}^{-1}T_{1X}^{-2} - 4\pi^2 J^2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)} =$$

$$= 4\frac{P + Q(ix)}{R + S(ix)}$$

with

$$P = -x^2 + T_{2A}^{-2} + 3T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 2\pi^2 J^2$$

$$Q = -2T_{2A}^{-1} - 3T_{1X}^{-1}$$

$$R = 3(T_{2A}^{-1} + T_{1X}^{-1})x^2 - T_{2A}^{-3} - 3T_{2A}^{-2}T_{1X}^{-1} - 2T_{2A}^{-1}T_{1X}^{-2} - 4\pi^2 J^2\left(T_{2A}^{-1} + T_{1X}^{-1}\right)$$

$$S = -x^2 + 3T_{2A}^{-2} + 6T_{2A}^{-1}T_{1X}^{-1} + 2T_{1X}^{-2} + 4\pi^2 J^2$$

$$I(x) = 4\frac{PR + QSx^2}{R^2 + S^2x^2}\ (eq.S3)$$

Approximate solution around x=0:

$$4/f(ix)=\frac{(ix)^2-(ix)(2T_{2A}^{-1}+3T_{1X}^{-1})+T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2}{(ix)^3-3(T_{2A}^{-1}+T_{1X}^{-1})(ix)^2+(3T_{2A}^{-2}+6T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+4\pi^2J^2)(ix)-T_{2A}^{-3}-3T_{2A}^{-2}T_{1X}^{-1}-2T_{2A}^{-1}T_{1X}^{-2}-4\pi^2J^2\left(T_{2A}^{-1}+T_{1X}^{-1}\right)}$$

$$f(0)=-\frac{T_{2A}^{-3}+3T_{2A}^{-2}T_{1X}^{-1}+2T_{2A}^{-1}T_{1X}^{-2}+4\pi^2J^2\left(T_{2A}^{-1}+T_{1X}^{-1}\right)}{T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2}$$

$$f'(0)=\frac{(T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2)(3T_{2A}^{-2}+6T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+4\pi^2J^2)-(2T_{2A}^{-1}+3T_{1X}^{-1})(T_{2A}^{-3}+3T_{2A}^{-2}T_{1X}^{-1}+2T_{2A}^{-1}T_{1X}^{-2}+4\pi^2J^2\left(T_{2A}^{-1}+T_{1X}^{-1}\right))}{(T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2)^2}=$$

$$=\frac{4T_{1X}^{-4}+12T_{1X}^{-3}T_{2A}^{-1}+13T_{1X}^{-2}T_{2A}^{-2}+T_{1X}^{-1}(6T_{2A}^{-3}+4T_{2A}^{-1}\pi^2J^2)+T_{2A}^{-4}+2T_{2A}^{-2}\pi^2J^2+8\pi^4J^4}{(T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2)^2}$$

$\Rightarrow$

$$f(ix)\approx const.(ix-\frac{f(0)}{f'(0)})\approx const.(ix-\pi W)$$

$$\pi W\approx\frac{(T_{2A}^{-3}+3T_{2A}^{-2}T_{1X}^{-1}+2T_{2A}^{-1}T_{1X}^{-2}+4\pi^2J^2\left(T_{2A}^{-1}+T_{1X}^{-1}\right))(T_{2A}^{-2}+3T_{2A}^{-1}T_{1X}^{-1}+2T_{1X}^{-2}+2\pi^2J^2)}{4T_{1X}^{-4}+12T_{1X}^{-3}T_{2A}^{-1}+13T_{1X}^{-2}T_{2A}^{-2}+T_{1X}^{-1}(6T_{2A}^{-3}+4T_{2A}^{-1}\pi^2J^2)+T_{2A}^{-4}+2T_{2A}^{-2}\pi^2J^2+8\pi^4J^4}=$$

$$=\frac{4T_{1X}^{-4}T_{2A}^{-1}+T_{1X}^{-3}(12T_{2A}^{-2}+8\pi^2J^2)+T_{1X}^{-2}(13T_{2A}^{-3}+24T_{2A}^{-1}\pi^2J^2)+T_{1X}^{-1}(6T_{2A}^{-4}+22T_{2A}^{-2}\pi^2J^2+8\pi^4J^4)+T_{2A}^{-5}+6T_{2A}^{-3}\pi^2J^2+8T_{2A}^{-1}\pi^4J^4}{4T_{1X}^{-4}+12T_{1X}^{-3}T_{2A}^{-1}+13T_{1X}^{-2}T_{2A}^{-2}+T_{1X}^{-1}(6T_{2A}^{-3}+4T_{2A}^{-1}\pi^2J^2)+T_{2A}^{-4}+2T_{2A}^{-2}\pi^2J^2+8\pi^4J^4}=$$

$$=\frac{4T_{2A}^{-1}+T_{1X}(12T_{2A}^{-2}+8\pi^2J^2)+T_{1X}^{2}(13T_{2A}^{-3}+24T_{2A}^{-1}\pi^2J^2)+T_{1X}^{3}(6T_{2A}^{-4}+22T_{2A}^{-2}\pi^2J^2+8\pi^4J^4)+T_{1X}^{4}(T_{2A}^{-5}+6T_{2A}^{-3}\pi^2J^2+8T_{2A}^{-1}\pi^4J^4)}{4+12T_{1X}T_{2A}^{-1}+13T_{1X}^{2}T_{2A}^{-2}+T_{1X}^{3}(6T_{2A}^{-3}+4T_{2A}^{-1}\pi^2J^2)+T_{1X}^{4}(T_{2A}^{-4}+2T_{2A}^{-2}\pi^2J^2+8\pi^4J^4)}=$$

$$=\frac{4T_{1X}^{-4}T_{2A}^{-1}+12T_{1X}^{-3}T_{2A}^{-2}+13T_{1X}^{-2}T_{2A}^{-3}+6T_{1X}^{-1}T_{2A}^{-4}+T_{2A}^{-5}+(8T_{1X}^{-3}+24T_{1X}^{-2}T_{2A}^{-1}+22T_{1X}^{-1}T_{2A}^{-2}+6T_{2A}^{-3})\pi^2J^2+8(T_{1X}^{-1}+T_{2A}^{-1})\pi^4J^4}{4T_{1X}^{-4}+12T_{1X}^{-3}T_{2A}^{-1}+13T_{1X}^{-2}T_{2A}^{-2}+6T_{1X}^{-1}T_{2A}^{-3}+T_{2A}^{-4}+(4T_{1X}^{-1}T_{2A}^{-1}+2T_{2A}^{-2})\pi^2J^2+8\pi^4J^4}=$$

$$=\frac{4T_{2A}^{-1}(T_{1X}^{-1}+T_{2A}^{-1})^4-4T_{2A}^{-2}(T_{1X}^{-1}+T_{2A}^{-1})^3+2T_{2A}^{-3}(T_{1X}^{-1}+T_{2A}^{-1})^2+(8(T_{1X}^{-1}+T_{2A}^{-1})^3-2T_{2A}^{-2}(T_{1X}^{-1}+T_{2A}^{-1}))\pi^2J^2+8(T_{1X}^{-1}+T_{2A}^{-1})\pi^4J^4}{4(T_{1X}^{-1}+T_{2A}^{-1})^4-4T_{2A}^{-1}(T_{1X}^{-1}+T_{2A}^{-1})^3+2T_{2A}^{-2}(T_{1X}^{-1}+T_{2A}^{-1})^2+(4T_{1X}^{-1}T_{2A}^{-1}+2T_{2A}^{-2})\pi^2J^2+8\pi^4J^4}$$

Taylor expansion in $\pi^2 J^2$:

$$\pi W \approx T_{2A}^{-1} + \frac{(4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4})(8T_{1X}^{-3} + 24T_{1X}^{-2}T_{2A}^{-1} + 22T_{1X}^{-1}T_{2A}^{-2} + 6T_{2A}^{-3}) - (4T_{1X}^{-1}T_{2A}^{-1} + 2T_{2A}^{-2})(4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4})T_{2A}^{-1}}{(4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4})^2}\pi^2 J^2 =$$

$$= T_{2A}^{-1} + \frac{(4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4})(8T_{1X}^{-3} + 24T_{1X}^{-2}T_{2A}^{-1} + 22T_{1X}^{-1}T_{2A}^{-2} + 6T_{2A}^{-3} - 4T_{1X}^{-1}T_{2A}^{-2} - 2T_{2A}^{-3})}{(4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4})^2}\pi^2 J^2 =$$

$$= T_{2A}^{-1} + \frac{8T_{1X}^{-3} + 24T_{1X}^{-2}T_{2A}^{-1} + 18T_{1X}^{-1}T_{2A}^{-2} + 4T_{2A}^{-3}}{4T_{1X}^{-4} + 12T_{1X}^{-3}T_{2A}^{-1} + 13T_{1X}^{-2}T_{2A}^{-2} + 6T_{1X}^{-1}T_{2A}^{-3} + T_{2A}^{-4}}\pi^2 J^2 =$$

$$= T_{2A}^{-1} + \frac{2(2T_{1X}^{-1} + T_{2A}^{-1})^2 (T_{1X}^{-1} + 2T_{2A}^{-1})}{(2T_{1X}^{-1} + T_{2A}^{-1})^2 (T_{1X}^{-1} + T_{2A}^{-1})^2}\pi^2 J^2 = T_{2A}^{-1} + 2\frac{T_{1X}^{-1} + 2T_{2A}^{-1}}{(T_{1X}^{-1} + T_{2A}^{-1})^2}\pi^2 J^2$$

Again, this approximation over-estimates the width.

<u>Quartet Case:</u>

$$A=\begin{bmatrix} ix+3\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & \frac{3}{2}T_{1X}^{-1} & 0 & 0 \\ \frac{1}{2}T_{1X}^{-1} & ix+\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & T_{1X}^{-1} & 0 \\ 0 & T_{1X}^{-1} & ix-\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & \frac{1}{2}T_{1X}^{-1} \\ 0 & 0 & \frac{3}{2}T_{1X}^{-1} & ix-3\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} \end{bmatrix}$$

$$x=2\pi(\nu-\nu_0)$$

$$\begin{aligned}
&|A|=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}+3\pi Ji)((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}-3\pi Ji)((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+\pi^2J^2-T_{1X}^{-2}) \\
&-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}+\pi Ji))-\tfrac{3}{4}T_{1X}^{-2}((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}-\pi Ji)(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}-3\pi Ji)-\tfrac{3}{4}T_{1X}^{-2})= \\
&=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}+3\pi Ji)((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+(\pi^2J^2-T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}) \\
&-3\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-3\pi Ji(\pi^2J^2-T_{1X}^{-2})-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2}\pi Ji) \\
&-\tfrac{3}{4}T_{1X}^{-2}((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-4\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-3\pi^2J^2-\tfrac{3}{4}T_{1X}^{-2})= \\
&=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^4+(\pi^2J^2-T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-3\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3 \\
&-3\pi Ji(\pi^2J^2-T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-\tfrac{3}{4}T_{1X}^{-2}\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}) \\
&+3\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+3\pi Ji(\pi^2J^2-T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+9\pi^2J^2(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2 \\
&+9\pi^2J^2(\pi^2J^2-T_{1X}^{-2})-\tfrac{9}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})\pi Ji+\tfrac{9}{4}T_{1X}^{-2}\pi^2J^2-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2 \\
&+3T_{1X}^{-2}\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{9}{4}T_{1X}^{-2}\pi^2J^2+\tfrac{9}{16}T_{1X}^{-4}= \\
&=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^4+(-3\pi Ji+3\pi Ji)(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3 \\
&+(\pi^2J^2-T_{1X}^{-2}-\tfrac{3}{4}T_{1X}^{-2}+9\pi^2J^2-\tfrac{3}{4}T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2 \\
&+(-3\pi Ji\pi^2J^2+3\pi JiT_{1X}^{-2}-\tfrac{3}{4}T_{1X}^{-2}\pi Ji+3\pi Ji\pi^2J^2-3\pi JiT_{1X}^{-2}-\tfrac{9}{4}\pi JiT_{1X}^{-2}+3T_{1X}^{-2}\pi Ji)(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1}) \\
&+9\pi^4J^4-9\pi^2J^2T_{1X}^{-2}+\tfrac{9}{4}T_{1X}^{-2}\pi^2J^2+\tfrac{9}{4}T_{1X}^{-2}\pi^2J^2+\tfrac{9}{16}T_{1X}^{-4}= \\
&=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^4+(10\pi^2J^2-\tfrac{5}{2}T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^4J^4-\tfrac{9}{2}T_{1X}^{-2}\pi^2J^2+\tfrac{9}{16}T_{1X}^{-4}= \\
&=(ix)^4-(ix)^3(4T_{2A}^{-1}+6T_{1X}^{-1})+(ix)^2(6T_{2A}^{-2}+18T_{2A}^{-1}T_{1X}^{-1}+\tfrac{27}{2}T_{1X}^{-2}+10\pi^2J^2-\tfrac{5}{2}T_{1X}^{-2}) \\
&-(ix)(4T_{2A}^{-3}+18T_{2A}^{-2}T_{1X}^{-1}+27T_{2A}^{-1}T_{1X}^{-2}+\tfrac{27}{2}T_{1X}^{-3}+20T_{2A}^{-1}\pi^2J^2+30T_{1X}^{-1}\pi^2J^2-5T_{2A}^{-1}T_{1X}^{-2}-\tfrac{15}{2}T_{1X}^{-3}) \\
&+T_{2A}^{-4}+6T_{2A}^{-3}T_{1X}^{-1}+\tfrac{27}{2}T_{2A}^{-2}T_{1X}^{-2}+\tfrac{27}{2}T_{2A}^{-1}T_{1X}^{-3}+\tfrac{81}{16}T_{1X}^{-4}-\tfrac{5}{2}T_{2A}^{-2}T_{1X}^{-2}-\tfrac{15}{2}T_{2A}^{-1}T_{1X}^{-3}-\tfrac{45}{8}T_{1X}^{-4}+\tfrac{9}{16}T_{1X}^{-4} \\
&+10T_{2A}^{-2}\pi^2J^2+30T_{2A}^{-1}T_{1X}^{-1}\pi^2J^2+\tfrac{45}{2}T_{1X}^{-2}\pi^2J^2+9\pi^4J^4-\tfrac{9}{2}T_{1X}^{-2}\pi^2J^2= \\
&=(ix)^4-(ix)^3(4T_{2A}^{-1}+6T_{1X}^{-1})+(ix)^2(6T_{2A}^{-2}+18T_{2A}^{-1}T_{1X}^{-1}+11T_{1X}^{-2}+10\pi^2J^2) \\
&-(ix)(4T_{2A}^{-3}+18T_{2A}^{-2}T_{1X}^{-1}+22T_{2A}^{-1}T_{1X}^{-2}+6T_{1X}^{-3}+20T_{2A}^{-1}\pi^2J^2+30T_{1X}^{-1}\pi^2J^2) \\
&+T_{2A}^{-4}+6T_{2A}^{-3}T_{1X}^{-1}+11T_{2A}^{-2}T_{1X}^{-2}+6T_{2A}^{-1}T_{1X}^{-3}+10T_{2A}^{-2}\pi^2J^2+30T_{2A}^{-1}T_{1X}^{-1}\pi^2J^2+18T_{1X}^{-2}\pi^2J^2+9\pi^4J^4
\end{aligned}$$

$$A=\begin{bmatrix} ix+3\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & \frac{3}{2}T_{1X}^{-1} & 0 & 0 \\ \frac{1}{2}T_{1X}^{-1} & ix+\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & T_{1X}^{-1} & 0 \\ 0 & T_{1X}^{-1} & ix-\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} & \frac{1}{2}T_{1X}^{-1} \\ 0 & 0 & \frac{3}{2}T_{1X}^{-1} & ix-3\pi Ji-T_{2A}^{-1}-\frac{3}{2}T_{1X}^{-1} \end{bmatrix}$$

$$A^{-1}=$$

$$=\frac{\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}}{|A|}$$

$$I(x)=\mathrm{Re}\{W\bullet A^{-1}\bullet 1\}$$

$$W\bullet A^{-1}\bullet 1=\begin{pmatrix}1\\3\\3\\1\end{pmatrix}\bullet A^{-1}\bullet\begin{pmatrix}1\\1\\1\\1\end{pmatrix}=$$

$$=\frac{A_{11}+A_{44}+A_{12}+A_{43}+A_{13}+A_{42}+A_{14}+A_{41}+3(A_{21}+A_{34}+A_{22}+A_{33}+A_{23}+A_{32}+A_{24}+A_{31})}{|A|}$$

$$A_{11}=(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+\pi^2J^2-T_{1X}^{-2})$$
$$-\tfrac{3}{4}T_{1X}^{-2}(ix+\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+(\pi^2J^2-T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-3\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2$$
$$-3\pi^3J^3i+3\pi JiT_{1X}^{-2}-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2}\pi Ji=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3-3\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+(\pi^2J^2-\tfrac{7}{4}T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})$$
$$-3\pi^3J^3i+\tfrac{9}{4}\pi JiT_{1X}^{-2}$$
$$A_{12}=-\tfrac{3}{2}T_{1X}^{-1}((ix-\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2})=$$
$$-\tfrac{3}{2}T_{1X}^{-1}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+6T_{1X}^{-1}\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{9}{2}\pi^2J^2T_{1X}^{-1}+\tfrac{9}{8}T_{1X}^{-3}$$
$$A_{13}=\tfrac{3}{2}T_{1X}^{-2}(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=\tfrac{3}{2}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{9}{2}T_{1X}^{-2}\pi Ji$$
$$A_{14}=-\tfrac{3}{4}T_{1X}^{-3}$$

$$A_{21}=-\tfrac{1}{2}T_{1X}^{-1}((ix-\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2})=$$
$$-\tfrac{1}{2}T_{1X}^{-1}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+2T_{1X}^{-1}\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{3}{2}\pi^2J^2T_{1X}^{-1}+\tfrac{3}{8}T_{1X}^{-3}$$
$$A_{22}=(ix-\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^2J^2)-\tfrac{3}{4}T_{1X}^{-2}(ix+3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+9\pi^2J^2(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-9\pi^3J^3i$$
$$-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{9}{4}T_{1X}^{-2}\pi Ji=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3-\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+(9\pi^2J^2-\tfrac{3}{4}T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})$$
$$-9\pi^3J^3i-\tfrac{9}{4}\pi JiT_{1X}^{-2}$$
$$A_{23}=-T_{1X}^{-1}((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^2J^2)=-T_{1X}^{-1}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-9T_{1X}^{-1}\pi^2J^2$$
$$A_{24}=\tfrac{1}{2}T_{1X}^{-2}(ix+3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=\tfrac{1}{2}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{3}{2}T_{1X}^{-2}\pi Ji$$

$$A_{31}=\tfrac{1}{2}T_{1X}^{-2}(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=\tfrac{1}{2}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{2}T_{1X}^{-2}\pi Ji$$
$$A_{32}=-T_{1X}^{-1}((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^2J^2)=-T_{1X}^{-1}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-9T_{1X}^{-1}\pi^2J^2$$
$$A_{33}=(ix+\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})((ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^2J^2)-\tfrac{3}{4}T_{1X}^{-2}(ix-3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+9\pi^2J^2(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+9\pi^3J^3i$$
$$-\tfrac{3}{4}T_{1X}^{-2}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{9}{4}T_{1X}^{-2}\pi Ji=$$
$$=(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^3+\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2+(9\pi^2J^2-\tfrac{3}{4}T_{1X}^{-2})(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})$$
$$+9\pi^3J^3i+\tfrac{9}{4}\pi JiT_{1X}^{-2}$$
$$A_{34}=-\tfrac{1}{2}T_{1X}^{-1}((ix+\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})(ix+3\pi Ji-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})-\tfrac{3}{4}T_{1X}^{-2})=$$
$$-\tfrac{1}{2}T_{1X}^{-1}(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})^2-2T_{1X}^{-1}\pi Ji(ix-T_{2A}^{-1}-\tfrac{3}{2}T_{1X}^{-1})+\tfrac{3}{2}\pi^2J^2T_{1X}^{-1}+\tfrac{3}{8}T_{1X}^{-3}$$

$$A_{41} = -\tfrac{3}{4} T_{1X}^{-3}$$
$$A_{42} = \tfrac{3}{2} T_{1X}^{-2} (ix + 3\pi Ji - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) = \tfrac{3}{2} T_{1X}^{-2} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) + \tfrac{9}{2} T_{1X}^{-2} \pi Ji$$
$$A_{43} = -\tfrac{3}{2} T_{1X}^{-1} ((ix + \pi Ji - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})(ix + 3\pi Ji - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) - \tfrac{3}{4} T_{1X}^{-2}) =$$
$$-\tfrac{3}{2} T_{1X}^{-1} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 - 6T_{1X}^{-1} \pi Ji (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) + \tfrac{9}{2} \pi^2 J^2 T_{1X}^{-1} + \tfrac{9}{8} T_{1X}^{-3}$$
$$A_{44} = (ix + 3\pi Ji - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})((ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 + \pi^2 J^2 - T_{1X}^{-2})$$
$$-\tfrac{3}{4} T_{1X}^{-2} (ix - \pi Ji - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) =$$
$$= (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^3 + (\pi^2 J^2 - T_{1X}^{-2})(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) + 3\pi Ji (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2$$
$$+ 3\pi^3 J^3 i - 3\pi Ji T_{1X}^{-2} - \tfrac{3}{4} T_{1X}^{-2} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1}) + \tfrac{3}{4} T_{1X}^{-2} \pi Ji =$$
$$= (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^3 + 3\pi Ji (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 + (\pi^2 J^2 - \tfrac{7}{4} T_{1X}^{-2})(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$
$$+ 3\pi^3 J^3 i - \tfrac{9}{4} \pi Ji T$$

$$A_{11} + A_{44} = 2(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^3 + 2(\pi^2 J^2 - \tfrac{7}{4} T_{1X}^{-2})(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$
$$3(A_{22} + A_{33}) = 6(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^3 + 6(9\pi^2 J^2 - \tfrac{3}{4} T_{1X}^{-2})(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$

$$3(A_{21} + A_{34}) = -3T_{1X}^{-1} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 + 9\pi^2 J^2 T_{1X}^{-1} + \tfrac{9}{4} T_{1X}^{-3}$$
$$3(A_{23} + A_{32}) = -6T_{1X}^{-1} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 - 54 T_{1X}^{-1} \pi^2 J^2$$
$$A_{12} + A_{43} = -3T_{1X}^{-1} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2 + 9\pi^2 J^2 T_{1X}^{-1} + \tfrac{9}{4} T_{1X}^{-3}$$

$$A_{13} + A_{42} = 3T_{1X}^{-2} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$
$$3(A_{24} + A_{31}) = 3T_{1X}^{-2} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$

$$A_{14} + A_{41} = -\tfrac{3}{2} T_{1X}^{-3}$$

$$(W \bullet A^{-1} \bullet 1)|A| =$$
$$= A_{11} + A_{44} + A_{12} + A_{43} + A_{13} + A_{42} + A_{14} + A_{41} + 3(A_{21} + A_{34} + A_{22} + A_{33} + A_{23} + A_{32} + A_{24} + A_{31}) =$$
$$8(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^3$$
$$-12T_{1X}^{-1} (ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})^2$$
$$+ (56\pi^2 J^2 - 2T_{1X}^{-2})(ix - T_{2A}^{-1} - \tfrac{3}{2} T_{1X}^{-1})$$
$$-36 T_{1X}^{-1} \pi^2 J^2 + 3T_{1X}^{-3} =$$

$$= 8(ix)^3 - (ix)^2 (24T_{2A}^{-1} + 36T_{1X}^{-1} + 12T_{1X}^{-1})$$
$$+ (ix)(24T_{2A}^{-2} + 72T_{1X}^{-1}T_{2A}^{-1} + 54T_{1X}^{-2} + 24T_{1X}^{-1}T_{2A}^{-1} + 36T_{1X}^{-2} + 56\pi^2 J^2 - 2T_{1X}^{-2})$$
$$- 8T_{2A}^{-3} - 36T_{1X}^{-1}T_{2A}^{-2} - 54T_{1X}^{-2}T_{2A}^{-1} - 27T_{1X}^{-3} - 12T_{1X}^{-1}T_{2A}^{-2} - 36T_{1X}^{-2}T_{2A}^{-1} - 27T_{1X}^{-3} - 56\pi^2 J^2 T_{2A}^{-1} + 2T_{2A}^{-1}T_{1X}^{-2}$$
$$- 84\pi^2 J^2 T_{1X}^{-1} + 3T_{1X}^{-3} + 3T_{1X}^{-3} - 36\pi^2 J^2 T_{1X}^{-1} =$$
$$= 8(ix)^3 - (ix)^2 (24T_{2A}^{-1} + 48T_{1X}^{-1}) + (ix)(24T_{2A}^{-2} + 96T_{1X}^{-1}T_{2A}^{-1} + 88T_{1X}^{-2} + 56\pi^2 J^2)$$
$$- 8T_{2A}^{-3} - 48T_{1X}^{-1}T_{2A}^{-2} - 88T_{1X}^{-2}T_{2A}^{-1} - 48T_{1X}^{-3} - 56\pi^2 J^2 T_{2A}^{-1} - 120\pi^2 J^2 T_{1X}^{-1} =$$
$$= 8((ix)^3 - 3(ix)^2 (T_{2A}^{-1} + 2T_{1X}^{-1}) + (ix)(3T_{2A}^{-2} + 12T_{1X}^{-1}T_{2A}^{-1} + 11T_{1X}^{-2} + 7\pi^2 J^2)$$
$$- T_{2A}^{-3} - 6T_{1X}^{-1}T_{2A}^{-2} - 11T_{1X}^{-2}T_{2A}^{-1} - 6T_{1X}^{-3} - 7\pi^2 J^2 T_{2A}^{-1} - 15\pi^2 J^2 T_{1X}^{-1})$$

$$I(x) = \mathrm{Re}\{W \bullet A^{-1} \bullet 1\}$$
$$W \bullet A^{-1} \bullet 1 = 8 / f(ix)$$

$$= 8\frac{\begin{array}{l}(ix)^3 - 3(ix)^2 (T_{2A}^{-1} + 2T_{1X}^{-1}) + (ix)(3T_{2A}^{-2} + 12T_{1X}^{-1}T_{2A}^{-1} + 11T_{1X}^{-2} + 7\pi^2 J^2)\\ - T_{2A}^{-3} - 6T_{1X}^{-1}T_{2A}^{-2} - 11T_{1X}^{-2}T_{2A}^{-1} - 6T_{1X}^{-3} - 7\pi^2 J^2 T_{2A}^{-1} - 15\pi^2 J^2 T_{1X}^{-1}\end{array}}{\begin{array}{l}(ix)^4 - (ix)^3 (4T_{2A}^{-1} + 6T_{1X}^{-1}) + (ix)^2 (6T_{2A}^{-2} + 18T_{2A}^{-1}T_{1X}^{-1} + 11T_{1X}^{-2} + 10\pi^2 J^2)\\ - (ix)(4T_{2A}^{-3} + 18T_{2A}^{-2}T_{1X}^{-1} + 22T_{2A}^{-1}T_{1X}^{-2} + 6T_{1X}^{-3} + 20T_{2A}^{-1}\pi^2 J^2 + 30T_{1X}^{-1}\pi^2 J^2)\\ + T_{2A}^{-4} + 6T_{2A}^{-3}T_{1X}^{-1} + 11T_{2A}^{-2}T_{1X}^{-2} + 6T_{2A}^{-1}T_{1X}^{-3} + 10T_{2A}^{-2}\pi^2 J^2 + 30T_{2A}^{-1}T_{1X}^{-1}\pi^2 J^2 + 18T_{1X}^{-2}\pi^2 J^2 + 9\pi^4 J^4\end{array}} =$$

$$= 8\frac{P + Q(ix)}{R + S(ix)}$$

with

$$P = 3x^2 (T_{2A}^{-1} + 2T_{1X}^{-1}) - T_{2A}^{-3} - 6T_{1X}^{-1}T_{2A}^{-2} - 11T_{1X}^{-2}T_{2A}^{-1} - 6T_{1X}^{-3} - 7\pi^2 J^2 T_{2A}^{-1} - 15\pi^2 J^2 T_{1X}^{-1}$$
$$Q = -x^2 + 3T_{2A}^{-2} + 12T_{1X}^{-1}T_{2A}^{-1} + 11T_{1X}^{-2} + 7\pi^2 J^2$$
$$R = x^4 - x^2 (6T_{2A}^{-2} + 18T_{2A}^{-1}T_{1X}^{-1} + 11T_{1X}^{-2} + 10\pi^2 J^2)$$
$$+ T_{2A}^{-4} + 6T_{2A}^{-3}T_{1X}^{-1} + 11T_{2A}^{-2}T_{1X}^{-2} + 6T_{2A}^{-1}T_{1X}^{-3} + 10T_{2A}^{-2}\pi^2 J^2 + 30T_{2A}^{-1}T_{1X}^{-1}\pi^2 J^2 + 18T_{1X}^{-2}\pi^2 J^2 + 9\pi^4 J^4$$
$$S = x^2 (4T_{2A}^{-1} + 6T_{1X}^{-1}) - 4T_{2A}^{-3} - 18T_{2A}^{-2}T_{1X}^{-1} - 22T_{2A}^{-1}T_{1X}^{-2} - 6T_{1X}^{-3} - 20T_{2A}^{-1}\pi^2 J^2 - 30T_{1X}^{-1}\pi^2 J^2$$

$$I(x) = 8\frac{PR + QSx^2}{R^2 + S^2 x^2} (eq. S4)$$

Approximate solution around x=0:

$$f(0)=-\frac{T_{2A}^{-4}+6T_{2A}^{-3}T_{1X}^{-1}+11T_{2A}^{-2}T_{1X}^{-2}+6T_{2A}^{-1}T_{1X}^{-3}+10T_{2A}^{-2}\pi^2J^2+30T_{2A}^{-1}T_{1X}^{-1}\pi^2J^2+18T_{1X}^{-2}\pi^2J^2+9\pi^4J^4}{T_{2A}^{-3}+6T_{1X}^{-1}T_{2A}^{-2}+11T_{1X}^{-2}T_{2A}^{-1}+6T_{1X}^{-3}+7\pi^2J^2T_{2A}^{-1}+15\pi^2J^2T_{1X}^{-1}}$$

$$f'(0)=\frac{\begin{aligned}&(T_{2A}^{-3}+6T_{1X}^{-1}T_{2A}^{-2}+11T_{1X}^{-2}T_{2A}^{-1}+6T_{1X}^{-3}+7\pi^2J^2T_{2A}^{-1}+15\pi^2J^2T_{1X}^{-1})(4T_{2A}^{-3}+18T_{2A}^{-2}T_{1X}^{-1}+22T_{2A}^{-1}T_{1X}^{-2}\\&+6T_{1X}^{-3}+20T_{2A}^{-1}\pi^2J^2+30T_{1X}^{-1}\pi^2J^2)-(T_{2A}^{-4}+6T_{2A}^{-3}T_{1X}^{-1}+11T_{2A}^{-2}T_{1X}^{-2}+6T_{2A}^{-1}T_{1X}^{-3}+10T_{2A}^{-2}\pi^2J^2\\&+30T_{2A}^{-1}T_{1X}^{-1}\pi^2J^2+18T_{1X}^{-2}\pi^2J^2+9\pi^4J^4)(3T_{2A}^{-2}+12T_{1X}^{-1}T_{2A}^{-1}+11T_{1X}^{-2}+7\pi^2J^2)\end{aligned}}{(T_{2A}^{-3}+6T_{1X}^{-1}T_{2A}^{-2}+11T_{1X}^{-2}T_{2A}^{-1}+6T_{1X}^{-3}+7\pi^2J^2T_{2A}^{-1}+15\pi^2J^2T_{1X}^{-1})^2}=$$

$$=\frac{\begin{aligned}&36T_{1X}^{-6}+132T_{1X}^{-5}T_{2A}^{-1}+193T_{1X}^{-4}T_{2A}^{-2}+144T_{1X}^{-3}T_{2A}^{-3}+58T_{1X}^{-2}T_{2A}^{-4}+12T_{1X}^{-1}T_{2A}^{-5}+T_{2A}^{-6}\\&+72T_{1X}^{-4}\pi^2J^2+234T_{1X}^{-3}T_{2A}^{-1}\pi^2J^2+223T_{1X}^{-2}T_{2A}^{-2}\pi^2J^2+84T_{1X}^{-1}T_{2A}^{-3}\pi^2J^2+11T_{2A}^{-4}\pi^2J^2\\&+225T_{1X}^{-2}\pi^4J^4+192T_{1X}^{-1}T_{2A}^{-1}\pi^4J^4+43T_{2A}^{-2}\pi^4J^4-63\pi^6J^6\end{aligned}}{(T_{2A}^{-3}+6T_{1X}^{-1}T_{2A}^{-2}+11T_{1X}^{-2}T_{2A}^{-1}+6T_{1X}^{-3}+7\pi^2J^2T_{2A}^{-1}+15\pi^2J^2T_{1X}^{-1})^2}$$

$\Rightarrow$

$$f(ix) \approx const.(ix - \frac{f(0)}{f'(0)}) \approx const.(ix - \pi W)$$

$$\pi W \approx \frac{\begin{array}{l}(T_{2A}^{-4} + 6T_{2A}^{-3}T_{1X}^{-1} + 11T_{2A}^{-2}T_{1X}^{-2} + 6T_{2A}^{-1}T_{1X}^{-3} + 10T_{2A}^{-2}\pi^2 J^2 + 30T_{2A}^{-1}T_{1X}^{-1}\pi^2 J^2 + 18T_{1X}^{-2}\pi^2 J^2 + 9\pi^4 J^4)\\ (T_{2A}^{-3} + 6T_{1X}^{-1}T_{2A}^{-2} + 11T_{1X}^{-2}T_{2A}^{-1} + 6T_{1X}^{-3} + 7\pi^2 J^2 T_{2A}^{-1} + 15\pi^2 J^2 T_{1X}^{-1})\end{array}}{\begin{array}{l}36T_{1X}^{-6} + 132T_{1X}^{-5}T_{2A}^{-1} + 193T_{1X}^{-4}T_{2A}^{-2} + 144T_{1X}^{-3}T_{2A}^{-3} + 58T_{1X}^{-2}T_{2A}^{-4} + 12T_{1X}^{-1}T_{2A}^{-5} + T_{2A}^{-6}\\ + 72T_{1X}^{-4}\pi^2 J^2 + 234T_{1X}^{-3}T_{2A}^{-1}\pi^2 J^2 + 223T_{1X}^{-2}T_{2A}^{-2}\pi^2 J^2 + 84T_{1X}^{-1}T_{2A}^{-3}\pi^2 J^2 + 11T_{2A}^{-4}\pi^2 J^2\\ + 225T_{1X}^{-2}\pi^4 J^4 + 192T_{1X}^{-1}T_{2A}^{-1}\pi^4 J^4 + 43T_{2A}^{-2}\pi^4 J^4 - 63\pi^6 J^6\end{array}} =$$

$$= \frac{\begin{array}{l}36T_{1X}^{-6}T_{2A}^{-1} + T_{1X}^{-5}(132T_{2A}^{-2} + 108\pi^2 J^2) + T_{1X}^{-4}(193T_{2A}^{-3} + 468T_{2A}^{-1}\pi^2 J^2)\\ + T_{1X}^{-3}(144T_{2A}^{-4} + 705T_{2A}^{-2}\pi^2 J^2 + 324\pi^4 J^4) + T_{1X}^{-2}(58T_{2A}^{-5} + 475T_{2A}^{-3}\pi^2 J^2 + 675T_{2A}^{-1}\pi^4 J^4)\\ + T_{1X}^{-1}(12T_{2A}^{-6} + 147T_{2A}^{-4}\pi^2 J^2 + 414T_{2A}^{-2}\pi^4 J^4 + 135\pi^6 J^6)\\ + T_{2A}^{-7} + 17T_{2A}^{-5}\pi^2 J^2 + 79T_{2A}^{-3}\pi^4 J^4 + 63T_{2A}^{-1}\pi^6 J^6\end{array}}{\begin{array}{l}36T_{1X}^{-6} + 132T_{1X}^{-5}T_{2A}^{-1} + 193T_{1X}^{-4}T_{2A}^{-2} + 144T_{1X}^{-3}T_{2A}^{-3} + 58T_{1X}^{-2}T_{2A}^{-4} + 12T_{1X}^{-1}T_{2A}^{-5} + T_{2A}^{-6}\\ + 72T_{1X}^{-4}\pi^2 J^2 + 234T_{1X}^{-3}T_{2A}^{-1}\pi^2 J^2 + 223T_{1X}^{-2}T_{2A}^{-2}\pi^2 J^2 + 84T_{1X}^{-1}T_{2A}^{-3}\pi^2 J^2 + 11T_{2A}^{-4}\pi^2 J^2\\ + 225T_{1X}^{-2}\pi^4 J^4 + 192T_{1X}^{-1}T_{2A}^{-1}\pi^4 J^4 + 43T_{2A}^{-2}\pi^4 J^4 - 63\pi^6 J^6\end{array}} =$$

$$= \frac{\begin{array}{l}36T_{2A}^{-1} + T_{1X}(132T_{2A}^{-2} + 108\pi^2 J^2) + T_{1X}^{2}(193T_{2A}^{-3} + 468T_{2A}^{-1}\pi^2 J^2)\\ + T_{1X}^{3}(144T_{2A}^{-4} + 705T_{2A}^{-2}\pi^2 J^2 + 324\pi^4 J^4) + T_{1X}^{4}(58T_{2A}^{-5} + 475T_{2A}^{-3}\pi^2 J^2 + 675T_{2A}^{-1}\pi^4 J^4)\\ + T_{1X}^{5}(12T_{2A}^{-6} + 147T_{2A}^{-4}\pi^2 J^2 + 414T_{2A}^{-2}\pi^4 J^4 + 135\pi^6 J^6)\\ + T_{1X}^{6}(T_{2A}^{-7} + 17T_{2A}^{-5}\pi^2 J^2 + 79T_{2A}^{-3}\pi^4 J^4 + 63T_{2A}^{-1}\pi^6 J^6)\end{array}}{\begin{array}{l}36 + 132T_{1X}T_{2A}^{-1} + T_{1X}^{2}(193T_{2A}^{-2} + 72\pi^2 J^2) + T_{1X}^{3}(144T_{2A}^{-3} + 234T_{2A}^{-1}\pi^2 J^2)\\ + T_{1X}^{4}(58T_{2A}^{-4} + 223T_{2A}^{-2}\pi^2 J^2 + 225\pi^4 J^4) + T_{1X}^{5}(12T_{2A}^{-5} + 84T_{2A}^{-3}\pi^2 J^2 + 192T_{2A}^{-1}\pi^4 J^4)\\ + T_{1X}^{6}(T_{2A}^{-6} + 11T_{2A}^{-4}\pi^2 J^2 + 43T_{2A}^{-2}\pi^4 J^4 - 63\pi^6 J^6)\end{array}}$$

$$= \frac{\begin{array}{l}1 + 12T_{1X}^{-1}T_{2A} + (17\pi^2 J^2 + 58T_{1X}^{-2})T_{2A}^{2} + 147T_{1X}^{-1}T_{2A}^{3}\pi^2 J^2 + 144T_{1X}^{-3}T_{2A}^{3}\\ + (79\pi^4 J^4 + 475T_{1X}^{-2}\pi^2 J^2 + 193T_{1X}^{-4})T_{2A}^{4} + (414T_{1X}^{-1}\pi^4 J^4 + 705T_{1X}^{-3}\pi^2 J^2 + 132T_{1X}^{-5})T_{2A}^{5}\\ + (468T_{1X}^{-4}\pi^2 J^2 + 63\pi^6 J^6 + 675T_{1X}^{-2}\pi^4 J^4 + 36T_{1X}^{-6})T_{2A}^{6}\\ + (135T_{1X}^{-1}\pi^6 J^6 + 324T_{1X}^{-3}\pi^4 J^4 + 108T_{1X}^{-5}\pi^2 J^2)T_{2A}^{7}\end{array}}{\begin{array}{l}1 + 12T_{1X}^{-1}T_{2A} + (58T_{1X}^{-2} + 11\pi^2 J^2)T_{2A}^{2} + (144T_{1X}^{-3} + 84T_{1X}^{-1}\pi^2 J^2)T_{2A}^{3}\\ + (43\pi^4 J^4 + 223T_{1X}^{-2}\pi^2 J^2 + 193T_{1X}^{-4})T_{2A}^{4} + (192T_{1X}^{-1}\pi^4 J^4 + 234T_{1X}^{-3}\pi^2 J^2 + 132T_{1X}^{-5})T_{2A}^{5}\\ + (72T_{1X}^{-4}\pi^2 J^2 + 36T_{1X}^{-6} + 225T_{1X}^{-2}\pi^4 J^4 - 63\pi^6 J^6)T_{2A}^{6}\end{array}} T_{2A}^{-1}$$

$$\pi W \approx \frac{\begin{array}{l}36T_{1X}^{-6}T_{2A}^{-1}+132T_{1X}^{-5}T_{2A}^{-2}+108T_{1X}^{-5}\pi^2J^2+193T_{1X}^{-4}T_{2A}^{-3}+468T_{1X}^{-4}T_{2A}^{-1}\pi^2J^2\\ +144T_{1X}^{-3}T_{2A}^{-4}+705T_{1X}^{-3}T_{2A}^{-2}\pi^2J^2+324T_{1X}^{-3}\pi^4J^4+58T_{1X}^{-2}T_{2A}^{-5}+475T_{1X}^{-2}T_{2A}^{-3}\pi^2J^2+675T_{1X}^{-2}T_{2A}^{-1}\pi^4J^4\\ +12T_{1X}^{-1}T_{2A}^{-6}+147T_{1X}^{-1}T_{2A}^{-4}\pi^2J^2+414T_{1X}^{-1}T_{2A}^{-2}\pi^4J^4+135T_{1X}^{-1}\pi^6J^6\\ +T_{2A}^{-7}+17T_{2A}^{-5}\pi^2J^2+79T_{2A}^{-3}\pi^4J^4+63T_{2A}^{-1}\pi^6J^6\end{array}}{\begin{array}{l}36T_{1X}^{-6}+132T_{1X}^{-5}T_{2A}^{-1}+193T_{1X}^{-4}T_{2A}^{-2}+144T_{1X}^{-3}T_{2A}^{-3}+58T_{1X}^{-2}T_{2A}^{-4}+12T_{1X}^{-1}T_{2A}^{-5}+T_{2A}^{-6}\\ +72T_{1X}^{-4}\pi^2J^2+234T_{1X}^{-3}T_{2A}^{-1}\pi^2J^2+223T_{1X}^{-2}T_{2A}^{-2}\pi^2J^2+84T_{1X}^{-1}T_{2A}^{-3}\pi^2J^2+11T_{2A}^{-4}\pi^2J^2\\ +225T_{1X}^{-2}\pi^4J^4+192T_{1X}^{-1}T_{2A}^{-1}\pi^4J^4+43T_{2A}^{-2}\pi^4J^4-63\pi^6J^6\end{array}} =$$

$$= \frac{\begin{array}{l}36T_{1X}^{-6}T_{2A}^{-1}+132T_{1X}^{-5}T_{2A}^{-2}+193T_{1X}^{-4}T_{2A}^{-3}+144T_{1X}^{-3}T_{2A}^{-4}+58T_{1X}^{-2}T_{2A}^{-5}+12T_{1X}^{-1}T_{2A}^{-6}+T_{2A}^{-7}\\ +(108T_{1X}^{-5}+468T_{1X}^{-4}T_{2A}^{-1}+705T_{1X}^{-3}T_{2A}^{-2}+475T_{1X}^{-2}T_{2A}^{-3}+147T_{1X}^{-1}T_{2A}^{-4}+17T_{2A}^{-5})\pi^2J^2\\ +(324T_{1X}^{-3}+675T_{1X}^{-2}T_{2A}^{-1}+414T_{1X}^{-1}T_{2A}^{-2}+79T_{2A}^{-3})\pi^4J^4\\ +(135T_{1X}^{-1}+63T_{2A}^{-1})\pi^6J^6\end{array}}{\begin{array}{l}36T_{1X}^{-6}+132T_{1X}^{-5}T_{2A}^{-1}+193T_{1X}^{-4}T_{2A}^{-2}+144T_{1X}^{-3}T_{2A}^{-3}+58T_{1X}^{-2}T_{2A}^{-4}+12T_{1X}^{-1}T_{2A}^{-5}+T_{2A}^{-6}\\ +(72T_{1X}^{-4}+234T_{1X}^{-3}T_{2A}^{-1}+223T_{1X}^{-2}T_{2A}^{-2}+84T_{1X}^{-1}T_{2A}^{-3}+11T_{2A}^{-4})\pi^2J^2\\ +(225T_{1X}^{-2}+192T_{1X}^{-1}T_{2A}^{-1}+43T_{2A}^{-2})\pi^4J^4-63\pi^6J^6\end{array}} =$$

Taylor expansion in $\pi^2 J^2$ gives:

$$\pi W \approx T_{2A}^{-1} + \frac{\begin{array}{l}108T_{1X}^{-5}+468T_{1X}^{-4}T_{2A}^{-1}+705T_{1X}^{-3}T_{2A}^{-2}+475T_{1X}^{-2}T_{2A}^{-3}+147T_{1X}^{-1}T_{2A}^{-4}+17T_{2A}^{-5}\\ -72T_{1X}^{-4}T_{2A}^{-1}-234T_{1X}^{-3}T_{2A}^{-2}-223T_{1X}^{-2}T_{2A}^{-3}-84T_{1X}^{-1}T_{2A}^{-4}-11T_{2A}^{-5}\end{array}}{36T_{1X}^{-6}+132T_{1X}^{-5}T_{2A}^{-1}+193T_{1X}^{-4}T_{2A}^{-2}+144T_{1X}^{-3}T_{2A}^{-3}+58T_{1X}^{-2}T_{2A}^{-4}+12T_{1X}^{-1}T_{2A}^{-5}+T_{2A}^{-6}}\pi^2J^2 =$$

$$= T_{2A}^{-1} + \frac{108T_{1X}^{-5}+396T_{1X}^{-4}T_{2A}^{-1}+471T_{1X}^{-3}T_{2A}^{-2}+252T_{1X}^{-2}T_{2A}^{-3}+63T_{1X}^{-1}T_{2A}^{-4}+6T_{2A}^{-5}}{36T_{1X}^{-6}+132T_{1X}^{-5}T_{2A}^{-1}+193T_{1X}^{-4}T_{2A}^{-2}+144T_{1X}^{-3}T_{2A}^{-3}+58T_{1X}^{-2}T_{2A}^{-4}+12T_{1X}^{-1}T_{2A}^{-5}+T_{2A}^{-6}}\pi^2J^2 =$$

$$= T_{2A}^{-1} + \frac{\begin{array}{l}108(T_{1X}^{-1}+T_{2A}^{-1})^5-144T_{2A}^{-1}(T_{1X}^{-1}+T_{2A}^{-1})^4-33T_{2A}^{-2}(T_{1X}^{-1}+T_{2A}^{-1})^3\\ +135T_{2A}^{-3}(T_{1X}^{-1}+T_{2A}^{-1})^2-72T_{2A}^{-4}(T_{1X}^{-1}+T_{2A}^{-1})+12T_{2A}^{-5}\end{array}}{\begin{array}{l}36(T_{1X}^{-1}+T_{2A}^{-1})^6-84T_{2A}^{-1}(T_{1X}^{-1}+T_{2A}^{-1})^5+73T_{2A}^{-2}(T_{1X}^{-1}+T_{2A}^{-1})^4\\ -28T_{2A}^{-3}(T_{1X}^{-1}+T_{2A}^{-1})^3+4T_{2A}^{-4}(T_{1X}^{-1}+T_{2A}^{-1})^2\end{array}}\pi^2J^2 \approx$$

$$\approx T_{2A}^{-1} + 3\frac{T_{1X}^{-1}+2T_{2A}^{-1}}{(T_{1X}^{-1}+T_{2A}^{-1})^2}\pi^2J^2$$

Again, this approximation over-estimates the width.

The least square fit of the apparent single peak to a Lorentz curve results in a peak narrower near the maximum than the actual signal. The solution above approximates the actual signal to a Lorentz peak near the peak maximum (x=0), thus the equations above always over-estimate the line width of the least square fit, but gives the functional shape of the expression (n=1,2,3):

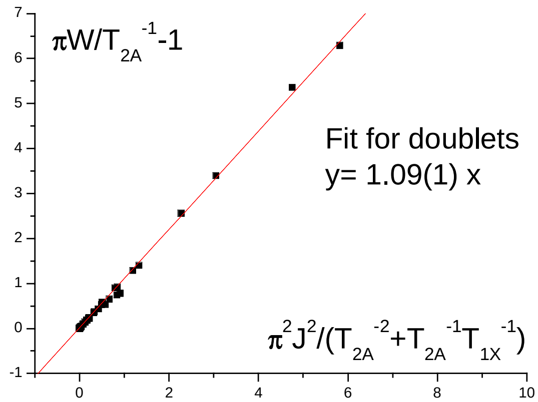
$$\pi W \approx T_{2A}^{-1} + n\frac{T_{1X}^{-1} + 2T_{2A}^{-1}}{(T_{1X}^{-1} + T_{2A}^{-1})^2}\pi^2 J^2$$

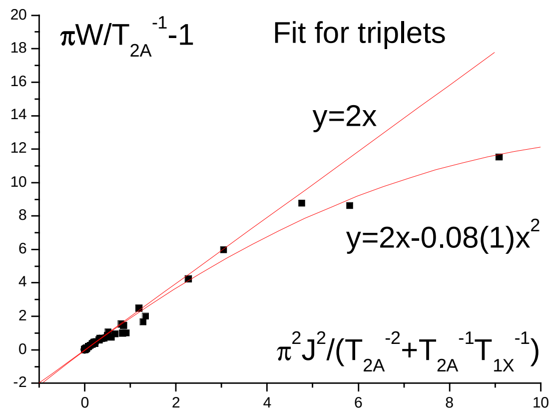
Least square fit to Lorentz peaks for the exact peak shape for the parameter ranges J from 3…300Hz, T_{1X}^{-1} from 100…2000Hz and T_{2A}^{-1} from 100…5000Hz should cover all reasonable values. All data can be fitted well to the following expression with n=1 for d, n=2 for t and n=3 for q:

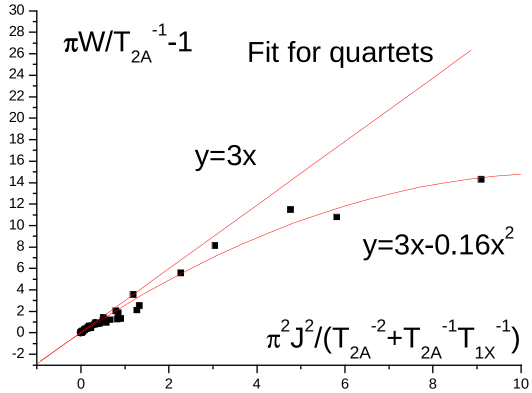
$$\pi W \approx T_{2A}^{-1} + n\frac{\pi^2 J^2}{T_{1X}^{-1} + T_{2A}^{-1}} (eq.4)$$

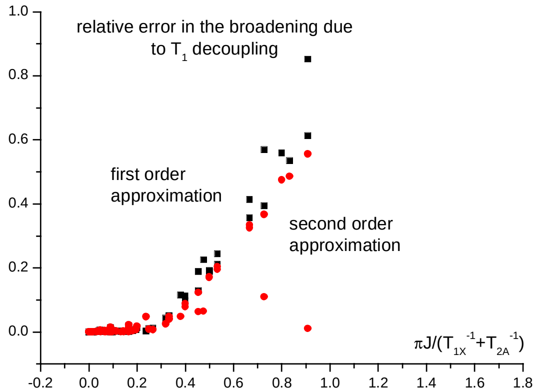
$$better:$$

$$\pi W \approx T_{2A}^{-1}[1 + n\frac{\pi^2 J^2}{(T_{1X}^{-1} + T_{2A}^{-1})T_{2A}^{-1}} - \frac{n-1}{4\pi}\left(\frac{\pi^2 J^2}{(T_{1X}^{-1} + T_{2A}^{-1})T_{2A}^{-1}}\right)^2](eq.S5)$$









In summary, the first order approximation is good within 5% for $J < (T_{1X}^{-1}+T_{2A}^{-1})/10$ and the second order approximation gives only slight improvement beyond this.

The first order approximation allows to propose the following general expression for the line width of a signal A with broadening after coalescence due to T_1 spin decoupling of several spin ½ nuclei X with coupling constants J_X and relaxation times T_{1X}:

$$\pi W_A \approx T_{2A}^{-1} + \sum_X \frac{\pi^2 J_X{}^2}{T_{1X}^{-1} + T_{2A}^{-1}} (eq.4)$$

Table 3: Linewidth W obtained from least square fitting of the curve calculated by eq.S1 (doublet), eq. S3 (triplet) and eq. S4 (quartet) to a single Lorentz peak and comparison to the approximations by eq.4 (FIT A)and eq.S5(second order)(FIT B):

πJ in Hz	T_{2A}^{-1} in Hz	T_{1X}^{-1} in Hz	W for d	d: FIT A	W for t	t: FIT A	t: FIT B	W for q	q: FIT A	q: FIT B
1000	1000	1000	486.7	477.5	586.5	636.6	630.3	669.5	795.8	783.1
800	1000	1000	428.2	420.2	505	522.0	519.4	568.9	623.9	618.7
500	1000	1000	362.1	358.1	399.7	397.9	397.5	433.1	437.7	436.9
100	1000	1000	320.1	319.9	321.8	321.5	321.5	323.6	323.1	323.1
10	1000	1000	318.328	318.3	318.345	318.3	318.3	318.363	318.4	318.4
--	--	--	--	--	--	--	--	--	--	--
1000	500	1000	381.9	371.4	477.5	583.6	561.1	563.2	795.7	750.7
800	500	1000	306.6	295.0	388.3	430.8	421.6	455.7	566.6	548.1
500	500	1000	218.4	212.2	264.3	265.3	263.9	303.3	318.3	315.5
100	500	1000	161.54	161.3	163.9	163.4	163.4	166.24	165.5	165.5
10	500	1000	159.179	159.2	159.203	159.2	159.4	159.227	159.2	159.2
--	--	--	--	--	--	--	--	--	--	--
1000	5000	1000	1647.1	1644.6	1699.1	1697.7	1697.5	1748.1	1750.7	1750.4
800	5000	1000	1627.2	1625.5	1661.3	1659.5	1659.4	1694.1	1693.4	1693.3
500	5000	1000	1605.5	1604.8	1619.2	1618.1	1618.1	1632.7	1631.3	1631.3
100	5000	1000	1592.11	1592.1	1592.67	1592.6	1592.6	1593.22	1593.1	1593.1
10	5000	1000	1591.555	1591.6	1591.561	1591.6	1591.6	1591.566	1591.6	1591.6
--	--	--	--	--	--	--	--	--	--	--
1000	100	1000	--	321.2	398.5	610.6	401.2	486.5	899.9	481.3
800	100	1000	232	217.0	306.2	402.2	316.5	374.8	587.4	415.9
500	100	1000	113.2	104.2	166.5	176.5	163.4	209.5	248.9	222.7
100	100	1000	34.94	34.72	38.02	37.62	37.60	41.06	40.51	40.47
10	100	1000	31.862	31.86	31.893	31.89	31.89	31.924	31.92	31.92
--	--	--	--	--	--	--	--	--	--	--
1000	1000	500000	318.947	318.9	319.583	319.6	319.6	320.22	320.2	320.2
800	1000	500000	318.717	318.7	319.125	319.1	319.1	319.532	319.5	319.5
500	1000	500000	318.469	318.5	318.628	318.6	318.6	318.787	318.8	318.8
100	1000	500000	318.316	318.3	318.323	318.3	318.3	318.329	318.3	318.3
10	1000	500000	318.31	318.3	318.31	318.3	318.3	318.31	318.3	318.3
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1000	1000	500	525.3	530.5	617.8	742.7	731.5	704.1	954.9	932.4
800	1000	500	455.7	454.1	533.5	589.9	585.3	599.8	725.7	716.5
500	1000	500	374.2	371.4	417.5	424.4	423.7	454.4	477.5	476.1
100	1000	500	320.6	320.4	322.86	322.6	322.5	325.1	324.7	324.7
10	1000	500	318.333	318.3	318.356	318.4	318.4	318.379	318.4	318.4
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1000	1000	2000	436.8	424.4	528.8	530.5	527.7	606.6	636.6	631.0
800	1000	2000	394.5	386.2	459	454.1	453.0	515.9	522.0	519.7
500	1000	2000	348.1	344.8	376.1	371.4	371.2	402.4	397.9	397.5
100	1000	2000	319.5	319.4	320.69	320.4	320.4	321.88	321.5	321.5
10	1000	2000	318.322	318.3	318.334	318.3	318.3	318.346	318.3	318.3
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1000	1000	100	565.7	607.7	637.1	897.1	876.1	735.9	1186.4	1144.6
800	1000	100	486.1	503.5	555.3	688.7	680.1	627.1	873.9	856.8
500	1000	100	388.7	390.7	434.9	463.0	461.7	474.3	535.3	532.7
100	1000	100	321.26	321.2	324.16	324.1	324.1	326.99	327.0	327.0
10	1000	100	318.339	318.3	318.369	318.4	318.4	318.399	318.4	318.4
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800	500	500	--	362.9	423.3	566.6	545.8	494.5	770.3	728.8
500	500	500	243.3	238.7	293.2	318.3	315.1	334.6	397.9	391.6
100	500	500	162.69	162.3	166.13	165.5	165.5	169.49	168.7	168.7
10	500	500	159.19	159.9	159.226	159.2	159.2	159.261	159.3	159.3
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1000	500	2000	302.2	286.5	403.5	413.8	405.7	486.7	541.1	524.9
800	500	2000	250.8	240.6	324.3	322.1	318.8	387.1	403.6	397.0
500	500	2000	194.8	191.0	227.6	222.8	222.3	258.1	254.6	253.0
100	500	2000	160.57	160.4	161.98	161.7	161.7	163.39	163.0	163.0
10	500	2000	159.169	159.2	159.183	159.2	159.2	159.197	159.2	159.2
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1000	500	100	--	689.7	--	1220.2	1079.5	--	1750.7	1469.3
800	500	100	--	498.7	--	838.2	780.6	--	1177.7	1062.5
500	500	100	277.3	291.8	316.6	424.4	415.6	363.4	557.0	539.5
100	500	100	164.64	164.5	169.76	169.8	169.8	174.59	175.1	175.0
10	500	100	159.21	159.2	159.265	159.3	159.3	159.321	159.3	159.3
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1000	5000	500	1651	1649.4	1706	1707.3	1707.1	1757.4	1765.2	1764.8
800	5000	500	1629.7	1628.5	1665.9	1665.6	1665.6	1700.6	1702.7	1702.5
500	5000	500	1606.5	1606.0	1621.1	1620.5	1620.5	1635.5	1635.0	1634.9
100	5000	500	1592.15	1592.1	1592.75	1592.7	1592.7	1593.34	1593.3	1593.3
10	5000	500	1591.555	1591.6	1591.561	1591.6	1591.6	1591.567	1591.6	1591.6
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1000	5000	2000	1640.5	1637.0	1687.1	1682.5	1682.4	1731.7	1728.0	1727.8
800	5000	2000	1622.9	1620.7	1653.3	1649.8	1649.7	1682.8	1678.9	1678.8
500	5000	2000	1603.83	1602.9	1615.96	1614.3	1614.3	1627.94	1625.7	1625.6
100	5000	2000	1592.041	1592.0	1592.533	1592.5	1592.5	1593.024	1592.9	1592.9
10	5000	2000	1591.554	1591.6	1591.559	1591.6	1591.6	1591.564	1591.6	1591.6
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1000	5000	100	1654.5	1654.0	1712	1716.4	1716.2	1765.5	1778.8	1778.4
800	5000	100	1631.9	1631.5	1670	1671.4	1671.4	1706.2	1711.4	1711.2
500	5000	100	1607.38	1607.2	1622.81	1622.8	1622.7	1637.97	1638.4	1638.3
100	5000	100	1592.184	1592.2	1592.818	1592.8	1592.8	1593.451	1593.4	1593.4
10	5000	100	1591.556	1591.6	1591.562	1591.6	1591.6	1591.568	1591.6	1591.6
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1000	100	2000	202.3	183.4	310.5	335.0	277.5	397.3	486.6	371.7
800	100	2000	139.8	128.8	222	225.8	202.3	289.8	322.9	275.8
500	100	2000	72.71	69.73	110.45	107.6	104.0	145.11	145.5	138.3
100	100	2000	33.412	33.35	34.991	34.86	34.86	36.567	36.38	36.37
10	100	2000	31.847	31.85	31.863	31.86	31.86	31.878	31.88	31.88
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100	100	500	37.73	37.14	43.32	42.44	42.37	48.64	47.75	47.61
10	100	500	31.89	31.88	31.948	31.94	31.94	32.007	32.00	32.00
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100	100	100	48.674	47.75	58.641	63.66	63.03	66.921	79.58	78.31
10	100	100	32.011	31.99	32.19	32.15	31.94	32.367	32.31	32.31