

The case of D2S: R.L.Cook, F.C.De Lucia, P.Helminger, J.Mol.Spectrosc. 41,123-136(1972)
 constants and errors have also been reproduced in Table 8.24, p.352 of the 3rd Edition of the Gordy and Cook textbook.

66 transitions in fit
 22 fitted constants (in the A-reduced asymmetric-rotor Hamiltonian in representation IIII)
 44 degrees of freedom

		as published	ASFIT ^a	PIFORM from all three SPFIT outputs 67%=sigma	SPFIT 0.05MHz errors	SPFIT 0.1MHz errors	SPFIT 0.2MHz errors
confidence level:		95% = 2sigma	67%=sigma				
A	/MHz	164571.118(45)	164571.118(22)	164571.118(22)	164571.1182(96)	164571.118(19)	164571.118(39)
B	/MHz	135380.313(45)	135380.313(22)	135380.313(22)	135380.3131(99)	135380.313(19)	135380.313(40)
C	/MHz	73244.068(71)	73244.067(29)	73244.067(29)	73244.067(12)	73244.067(25)	73244.068(51)
DJ	/MHz	13.0763(26)	13.0763(12)	13.0763(12)	13.07631(56)	13.0763(11)	13.0763(22)
DJK	/MHz	-41.7800(66)	-41.7799(33)	-41.7799(33)	-41.7799(14)	-41.7799(28)	-41.7800(58)
DK	/MHz	29.2170(113)	29.2170(56)	29.2170(56)	29.2170(24)	29.2170(49)	29.2170(98)
dJ	/MHz	-1.95725(68)	-1.95725(33)	-1.95725(33)	-1.95725(14)	-1.95725(29)	-1.95725(59)
dK	/MHz	47.2516(37)	47.2515(18)	47.2515(18)	47.25157(81)	47.2515(16)	47.2516(33)
HJ	/kHz	3.783(41)	3.782(20)	3.782(20)	3.7828(90)	3.782(18)	3.783(36)
HJK	/kHz	-32.06(20)	-32.06(10)	-32.061(98)	-32.061(43)	-32.061(86)	-32.061(172)
HKJ	/kHz	63.73(44)	63.73(22)	63.735(220)	63.735(96)	63.735(192)	63.730(380)
HK	/kHz	-36.20(75)	-36.20(37)	-36.200(378)	-36.200(163)	-36.200(330)	-36.200(650)
hJ	/kHz	-0.984(16)	-0.9836(77)	-0.9836(77)	-0.9836(34)	-0.9836(68)	-0.983(13)
hJK	/kHz	24.43(19)	24.428(93)	24.429(92)	24.429(41)	24.429(81)	24.429(163)
hK	/kHz	88.04(65)	88.04(33)	88.044(325)	88.04(14)	88.04(28)	88.04(57)
LJJK	/ Hz	27.47(101)	27.47(50)	27.47(50)	27.47(22)	27.47(44)	27.47(88)
LJK	/ Hz	-88.5(107)	-88.5(54)	-88.5(54)	-88.5(23)	-88.5(47)	-88.5(94)
LKKJ	/ Hz	78.(21)	77.7(106)	77.7(105)	77.7(46)	77.7(92)	77.7(185)
lJ	/ Hz	0.772(102)	0.772(50)	0.772(50)	0.772(22)	0.772(44)	0.772(89)
lJK	/ Hz	-17.50(131)	-17.50(66)	-17.50(65)	-17.50(29)	-17.50(57)	-17.50(115)
lK	/ Hz	-576.(25)	-576.(13)	-576.(13)	-576.0(55)	-576.(11)	-576.(22)
pK	/ Hz	1.95(32)	1.94(16)	1.94(15)	1.948(69)	1.94(13)	1.94(27)
s_fit	/MHz		0.114621 ^b		0.093588	0.093588	0.093588
RMS			1.146211 ^b		1.87175	0.93588	0.46794

a - ASFIT only allows to fit the IIIr and not the IIII Hamiltonian, so that the original signs of dJ,dK,hj,hjk,hk,etc.
 have been reversed to those consistent with the IIII fit.

b - worked out using N_degf=N_lines-N_const, otherwise only with N_lines.