

Table S9. Comparison of results of fitting the newly measured transition frequencies for the 2nu9 dyad in 35ClON02 with two different fitting schemes.

| 2nu9 dyad    | SPFIT index | new data, JMS2002 2v9 | scheme(modified) v7 | new scheme with fixed gs sextics 2v9 | v7             | 2v9 estimate from gs and v9=1 |
|--------------|-------------|-----------------------|---------------------|--------------------------------------|----------------|-------------------------------|
| A /MHz       | 100vv       | 11933.0077(72)        | 12116.9247(82)      | 11906.720(25)                        | 12143.309(23)  | 11903.50                      |
| B /MHz       | 200vv       | 2776.26461(21)        | 2771.27217(20)      | 2776.7359(12)                        | 2770.7929(11)  | 2776.628                      |
| C /MHz       | 300vv       | 2264.61090(17)        | 2251.95564(16)      | 2266.22014(35)                       | 2250.34576(35) | 2266.115                      |
| DJ /kHz      | 2vv         | 0.533140(27)          | 0.482773(26)        | 0.516077(20)                         | 0.499975(20)   | 0.51625                       |
| DJK /kHz     | 11vv        | 2.92717(84)           | 4.8375(10)          | 3.83003(22)                          | 3.92230(23)    | 3.8373                        |
| DK /kHz      | 20vv        | 18.577(40)            | -1.896(54)          | 7.188(19)                            | 10.683(20)     | 6.740                         |
| d1 /kHz      | 401vv       | -0.086337(27)         | -0.105647(26)       | -0.0956221(72)                       | -0.0964201(72) | -0.09593                      |
| d2 /kHz      | 500vv       | -0.019246(15)         | -0.016015(18)       | -0.0163485(60)                       | -0.0188995(69) | -0.01610                      |
| HJ /Hz       | 3vv         | -0.0003623(26)        | 0.0000742(25)^**    | [-0.0001362]                         | [-0.0001362]   |                               |
| HJK /Hz      | 12vv        | 0.01564(10)           | 0.4883(15)          | [-0.005812]                          | [-0.005812]    |                               |
| HKJ /Hz      | 21vv        | -0.5239(13)           | -0.021149(93)       | [-0.01504]                           | [-0.01504]     |                               |
| HK /Hz       | 30vv        | [ 0. ]^***            | -7.735(84)          | [ 0.03915]                           | [ 0.03915]     |                               |
| h1 /Hz       | 402vv       | 0.0003081(28)         | -0.0003428(27)      | [-0.00002388]                        | [-0.00002388]  |                               |
| h2 /Hz       | 501vv       | -0.0001770(21)        | 0.0001781(22)       | [-0.000004463]                       | [-0.000004463] |                               |
| h3 /Hz       | 600vv       | 0.00003300(68)        | -0.00003639(81)     | [ 0.000004716]                       | [ 0.000004716] |                               |
| LKJ /mHz     | 22vv        | 0.1187(12)            | 0.00769(13)         |                                      |                |                               |
| LKKJ /mHz    | 31vv        | -0.00741(11)          | -0.1225(13)         |                                      |                |                               |
| DE_0 =v7-2v9 | 11          |                       |                     | 411733.435(89000)                    |                |                               |
| DEeff        | 11          | 503806.77(30)         |                     | [ 503804.79(15)^* ]                  |                |                               |
| F+- /MHz     | 40001       |                       | -0.34115(56)        |                                      |                |                               |
| F+-J /MHz    | 40101       |                       | -0.00000634(15)     |                                      |                |                               |
| F+-K /MHz    | 41001       |                       | 0.0001004(33)       |                                      |                |                               |
| F+-JK /MHz   | 41101       |                       | 0.00000002410(90)   |                                      |                |                               |
| Gc /MHz      | 600001      |                       |                     | 335.977(21)                          |                |                               |
| GcJ /MHz     | 600101      |                       |                     | -0.0006434(26)                       |                |                               |
| GcK /MHz     | 601001      |                       |                     | -0.004261(59)                        |                |                               |
| Fab /MHz     | 610001      |                       | 5.183(22)           |                                      |                |                               |
| FabJ /MHz    | 610101      |                       | 0.00008129(83)      |                                      |                |                               |
| FabK /MHz    | 611001      |                       | -0.001476(20)       |                                      |                |                               |
| C3 /MHz      | 620001      |                       | -0.001924(40)       |                                      |                |                               |
| W_F /MHz     | 1           |                       |                     | 145167.871(63000)                    |                |                               |
| W_F^AJ /MHz  | 101         |                       |                     | -0.1138(25)                          |                |                               |
| W_F^AK /MHz  | 1001        |                       |                     | -8.0684(69)                          |                |                               |
| Nconst       |             | 42                    |                     | 23                                   |                |                               |
| Nlines       |             | 3800                  |                     | 3800                                 |                |                               |
| sigma /MHz   |             | 0.0614                |                     | 0.0453                               |                |                               |

\* Calculated from DE\_0 and W\_F by accounting for correlation coefficient C(DE\_0,W\_F)=-0.999998  
 \*\* fitted here and fixed in the original paper (J.Mol.Spectrosc. 213 (2002) 8-14 )  
 \*\*\* fixed here and fitted in the original paper.