Electronic supplementary material S4 to

High resolution spectroscopy of asymmetric top molecules in nonsinglet electronic states: The ν_3 fundamental of chlorine dioxide ($^{16}O^{35}Cl^{16}O$) free radical in the X^2B_1 electronic ground state

Nonzero matrix elements of the ${}^{(6)}H^v_{sp-rot}$ spin–rotational operator:

$$\begin{aligned}&\left\langle NK\gamma, SJ|{}^{(6)}H^v_{sp-rot}|NK\gamma, SJ\right\rangle = \{(H^s_{NNK}+H^s_{KNN})N^2(N+1)^2K^2\\&+(H^s_{NKK}+H^s_{KKN})K^4N(N+1)+H^s_KK^6+H^s_NN^3(N+1)^3\\&+\delta_{K,1}[(h^s_{KN}+h^s_{NK})+h^s_{NN}N(N+1)]N^2(N+1)^2(-1)^\gamma\}\\&\times\frac{N(N+1)-J(J+1)+S(S+1)}{2N(N+1)},\end{aligned}\tag{1}$$

$$\begin{aligned}&\left\langle NK\gamma, SJ|{}^{(6)}H^v_{sp-rot}|NK+\pm2\gamma, SJ\right\rangle = \frac{1}{4}\{(h^s_{KN}+h^s_{NK})[K^2+(K+\pm2)^2]\\&+2h^s_{NN}N(N+1)\}\{(1-\delta_{K,0})(1-\delta_{K,2}\delta_{\Delta K,-2})+\sqrt{2}(\delta_{K,0}+\delta_{K,2}\delta_{\Delta K,-2})\}\\&\times\{J(J+1)-N(N+1)-S(S+1)\}\\&\times\{(N\mp K)(N\pm K+1)(N\mp K-1)(N\pm K+2)\}^{1/2},\end{aligned}\tag{2}$$

$$\begin{aligned}&\left\langle N-1K\gamma, SJ|{}^{(6)}H^v_{sp-rot}|NK\gamma'\neq\gamma, SJ\right\rangle = -[H^s_KK^4+H^s_{NKK}K^2N^2\\&+H^s_{NNK}N^2(N+1)^2-2\delta_{K,1}(-1)^\gamma h^s_{NK}N^3]\\&\times\frac{K}{2N}\left\{\frac{(N^2-K^2)(N-J+S)(N+J+S+1)(S+J-N+1)(N+J-S)}{(2N-1)(2N+1)}\right\}^{1/2},\end{aligned}\tag{3}$$

$$\begin{aligned}&\left\langle N-1K\gamma, SJ|{}^{(6)}H^v_{sp-rot}|NK+\pm2\gamma'\neq\gamma, SJ\right\rangle\\&=-\frac{h^s_{Nk}}{4N}\{(K+\pm2)N(N-1)(N\mp K-2)+KN(N+1)(N\mp K)\}\\&\times[(1-\delta_{K,0})(1-\delta_{K,2}\delta_{\Delta K,-2})+\sqrt{2}(\delta_{K,0}+\delta_{K,2}\delta_{\Delta K,-2})]\\&\times\left\{\frac{(N\pm K+1)(N\mp K-1)(N\pm K)(N\pm K+2)}{(2N-1)(2N+1)}\right\}^{1/2}\\&\times\{(N-J+S)(N+J+S+1)(S+J-N+1)(N+J-S)\}^{1/2}.\end{aligned}\tag{4}$$