

**Table S3** Energy (in  $cm^{-1}$ ) in the first rovibrational levels ( $J \leq 6$ ,  $K=0,1,2$  and symmetry  $A_1$ ) for the  $O_2-O_2$  dimer in the quintet electronic state, calculated using the *helicity decoupling* approximation. The rotational constants are also reported.

| $K$ | $J = 0$   | $J = 1$   | $J = 2$   | $J = 3$   | $J = 4$   | $J = 5$   | $J = 6$   | rotational constant |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|---------------------|
| 0   | -93.17298 | -90.09667 | -92.72015 | -89.34656 | -91.66404 | -87.99745 | -90.00580 | 0.07525             |
|     | -73.59487 | -68.98990 | -73.15771 | -68.27593 | -72.13834 | -66.99195 | -70.53840 | 0.07222             |
|     | -66.10246 | -68.69159 | -65.66550 | -67.95707 | -64.64681 | -66.63691 | -63.04852 | 0.07301             |
|     | -65.82112 | -64.00624 | -65.39885 | -63.28009 | -64.41401 | -61.97360 | -62.86775 | 0.07124             |
|     | -63.39282 | -57.01120 | -62.96126 | -56.30379 | -61.95454 | -55.03175 | -60.37332 | 0.04142             |
| 1   |           | -89.88438 | -78.75209 | -89.13364 | -77.73503 | -87.78331 | -76.13884 | 0.07399             |
|     |           | -71.67347 | -72.04721 | -70.95931 | -71.04465 | -69.67510 | -69.47017 | 0.07148             |
|     |           | -67.02095 | -60.63819 | -66.30995 | -59.65239 | -65.03071 | -58.10517 | 0.07104             |
|     |           | -58.58453 | -57.26932 | -57.88209 | -56.26982 | -56.61947 | -54.70049 | 0.07078             |
|     |           | -56.20443 | -52.12096 | -55.49527 | -51.17426 | -54.21906 | -49.68866 | 0.06924             |
| 2   |           |           | -91.47265 | -77.35383 | -90.41877 | -76.00069 | -88.76403 | 0.07522             |
|     |           |           | -79.50049 | -66.92465 | -78.44173 | -65.64659 | -76.77928 | 0.07406             |
|     |           |           | -68.54424 | -58.63419 | -67.53591 | -57.34783 | -65.95302 | 0.07181             |
|     |           |           | -62.85282 | -51.13159 | -61.86103 | -49.86844 | -60.30408 | 0.07060             |
|     |           |           | -55.27640 | -46.60951 | -54.28656 | -45.34865 | -52.73268 | 0.07046             |