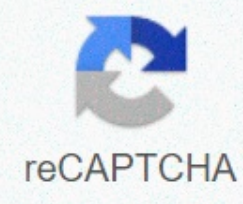




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# Maintenance engineering handbook

[illegible]



starts with a set of three peaks (b1-b3) at 29 308, 29 425, and 29 775 cm-1 (3.63, 3.65, and 3.69 eV). An area of several small low-intensity peaks reaches up to, ranging from peak b8 at 30 257 cm-1, the intensity of subsequent peaks increases. The strongest peak in BS2 at 30 931 cm-1 (b25, 3.83 eV) is a cross section of 14.5 Mb, so it is about eight times stronger than the most intense band in BS1 (a2). The total combined power of BS2 is about 20 times that of BS1. Several areas of closely related peaks are visible. The last clearly observed peak was observed at 32 289 cm-1 (b57, 4.00 eV). Au2+ Band System EPD Spectrum (BS2) is measured at a nozzle temperature of T = 120 K and the calculated transitions of all excited countries contributing to this energy range (lower board). The calculated spectrum varies by +1678 cm-1 and is folded with a Gaussian line profile with a FWHM of 10 cm-1. Experimental peaks (table S2 in SI) discussed in text are highlighted. The different colors on the calculated spectrum refer to transitions from the respected ES as specified in the legend. A more quantitative understanding of Spectra EPD is possible by comparing the results to high-level quantum chemical calculations combined with the simulations of vibronic spectra. As a result, we calculate the electronic states of Au2+ by using the average CASSCF (SA-CASSCF) method followed by internal cow interaction (MRCI) calculations as implemented in the MOLPRO.19 program package for the golden atom. The relatively efficient core potential of 19 electrons (MDF60) developed by Figgen et al.20 combined with the effective core potential (MDF60) developed by Figgen et al.20 combined with Figgen et.20's effective core potential combined with Figgen et.20's effective core potential combined with Figgen's effective core potential et.20 An atomic base kit is used in the contract.20 Then effects are included by the SO Hamiltonian diagonal on the basis of MRCI eigenstates using MDF60 SO-pseudodontial to represent the SO coupling operator. The active space for SA-CASSCF calculations consists of 10 sea routes derived from atomic 5D orbits and two Vallance orbits derived from the atomic orbits of the 6s. The core orbits of the 5 and 5 pence are kept frozen. The potential energy curves and transitional dipole moment components for all electronic countries are precalculated in a delicate grid extending from 2.1 to 7.1 Å. Cubic line interpolation is used to obtain continuous representation of the curves. The vibration eigenstates for each diabatic electronic mode are numerically calculated on a grid containing 512 points using a fertile representation of the kinetic energy operator. An electronic spectra that is solved in a simulated vibrational way starting with the Boltzmann population of the initial vibration modes in the ground electronic state at different temperatures. In order to calculate the strength of the spectral line, the moments of differentiation of transition between all initial and last pairs of countries are calculated through nomical integration and take into account the full dependence of the electronic transition dipole moments. By comparison, we will also complete time-dependent density functional theory (TD-DFT) calculations at the CAM-B3LYP/aug-cc-pVTZ.21 PESs levels calculated at different levels of the theory for the soil and excited electronic modes of Au2+ are shown in Figure 3. The atomic distance of the equilibrium in the ground state 2pg+ (GS) is calculated as re=2.64 Å at the MRCI-SO level with de=1.84 eV dissociation energy, Calculated as the difference of energies in re and r= 7.15 Å. This energy is lower than the recently calculated values and the experimental value of D0=2.21±0.21 eV.14 The CCSD-level calculated dissociation energy (T) is a value of De=1.98 eV (Fig. S4 in SI). By comparing Au2's experimental dissociation energy, D0=2.290±0.008 eV,8 to one of Au2+ and given that Au2+ has one electron less bonding than Au2, one would expect D0 to be at the low energy edge of the reported experimental range, as the CCSD level (T) predicted. Au2+ potential energy surfaces (PESs) at different levels of the theory. Red curves in (a) and (c) indicate states with non-strait sediate strength. Line-in (a) and (c) line curves indicate quartet states. While the calculated GSs PES are very similar for the three different theoretical models, we find big differences in the ES bar (Fig. 3). ES PESs below 3 eV of the TD-DFT and MRCI calculations that are not so-together (panels A and C) in Table 3) are similar in relative position (for lower ESs) and shape of the PESS band States. However, the absolute energies calculated with TD-DFT are 0.2-0.5 eV lower than those calculated using MRCI when the difference increases with higher lying situations. At higher energies, differences increase significantly and the relative order of countries changes. The second optically permitted transition calculated with MRCI that is not involved in SO-togetherness (2Mu) has a minimum 2.4 eV above the GS. The corresponding minimum calculated with TD-DFT occurs at eV 2.2. The lowest 4pg+ quartet of lies mode is found at 3.2 eV (2.7 eV in case of TD-DFT) above GS. Optically permitted transitions to 2Mu+, 2, and 2Mu countries calculated without SO coupling include vertical stimulation energies of 1.2, 2.4, and 3.7 eV, respectively (0.97, 1.98, and 3.48 eV for TD-DFT). If both 2 – 2+ and 2Mu – 2Mg+ transitions were the observed ones (2Mu+ – 2Üg+ is well below D0), then the calculations are 0.4 and 0.4 eV from the experiment, respectively. The calculated TD-DFT reconnamation strengths and pseudo-Frank-Condon progress also do not resemble the observed spectrum (Fig. S3 in SI). After so coupling is included, the image changes drastically (Figure 3, Table B). The first five stripes made up of several sets of ESs approach each other with energy. We find eight ESs in tight matuses between 2.8 and 3.2 eV derived from optically permitted countries with 2Mu+ symmetry and 2İİu mixed with the lowest quartet countries with 4Mg+ symmetry using SO coupling. In the range of BS2, we again find eight excited mani bystipes at close range derived from tight-range coupling quartet countries with symmetry 4pg+ and 4 4 4 000 with all double states lying close. The lower countries are inaccessible by a single puta EPD because they are all below D0. (Although some high-vibration lie countries may break away, the FC factors are probably low because GS and fifth ES PESs are very similar.) To enable a more detailed comparison with the experiment, we display the calculated line positions and strengths in letters 1 and 2. The calculated transitions in the BS1 range pass at -929 cm-1 to align the summit with the highest calculated intensity to the a2 peak. The different colors represent the different ESs in this range. Only countries that contribut significantly to power in this range are out of step. The calculated spectrum is approximately 0.25 eV, with the highest intense peaks occurring at lower energies. Numbered countries 17, 18, 21, 22 and 23 are responsible for most of the intensity. While the overall shape of the calculated spectrum is similar to the experimental one, we cannot allocate individual peaks easily. Peak a2 can be beyond state 17 and a10 may be beyond the state of 22 or 23. However, very small changes in PESs lead to relatively large changes Of the calculated peaks. The intensity calculated above 24 000 cm1 is mainly due to transitions to state 23. The gap between the calculated and experimental spectrum above 24,000 cm1 can be caused by an over-value of the intensity of the vases and the Frank-Condon factor of State 23. Plotting with letter 2 are the calculated strengths of the transitions in the BS2 energy range. They range by +1628 cm-1 (matching the position of the strongest peak from country 35 to the location of b25) and are listed according to the appropriate ES. Such a difference between theory and experiment is common in systems containing metal atoms even at the high level employed of the theory.22 Again, a peak one-on-one task cannot be performed. However, the overall contours and peak density are similar to the experimental spectrum. Although the intensities are not replicated, we can assume that b1-b3 are transitions to 31 due to the unique position at the low energy end of BS2. At least part of b25 is due to a transition to state 35 and the range of inflated peaks of similar intensity between 31 250 and 31 750 cm-1 (b35-b47) is caused by crossings to countries 35 and 36. Like BS1, we have calculated power on the high energy side of the spectrum that has not been experimentally observed. In conclusion, we can say that no TD-DFT nor non-SO-together MRCI calculations can predict the experimental spectrum of this seemingly simple diethomic ion. It is therefore essential to consider SO coupling to predict the location and shape of the band's observed systems. In conclusion, we present here the first absorption spectrum of au2+ isolated and compare the results to several theoretical models. The spectrum does not show a simple vibran structure with clear normal vibrational progression of individual excited modes as observed for example for Au2, which is a closed shell system.8b, 12 Instead, we observe two band systems with peak positions and seemingly irregular intensities. We show that the spectrum can be explained by strong SO coupling resulting in shifts of excited situation surfaces together. The observed band systems are caused by a number of well-polite excited situations, which make quantitative comprehension very challenging. In fact, while we can restore spectral shape and position and perhaps some of the many expected peaks, the method is still inaccurate enough to allow specific peaks to be assigned to vibrating passages. However, the electronic structure now seems well established and may provide deeper insight into the catalytic properties of Au2+ in the future. The high-resolution experimental data will enable further improvement (fine-tuning) of Au2+ PESs by making minor adjustments through transformation and/or algorithm matching which Will allow the experimental Weibron peaks to be fully allocated. Our results show that this simple diotomic ion with a single electron β(s) in a homo has a complex electronic structure that requires relative care and consideration of SO coupling. This work was supported by The Deutsche Forschungsgemeinschaft (DO 729/9) and OX/BER Research Partnership Seed Finance Fund. We admit A. Fielicke (TU Berlin) on providing pole target Au and S. R. Mackenzie (Oxford) for stimulating discussions. Open Access Funding is operated and organized by Projekt DEAL. The authors do not declare a conflict of interest. As a service to our authors and readers, this log provides supporting information provided by the authors. Such materials are reviewed by colleagues and reorganised for online delivery, but are not copies or values. Technical support issues arising from information support (except missing files) should be addressed to authors. Note: The publisher is not responsible for the content or functionality of any supporting information provided by the authors. Queries (other than missing content) should be directed to the appropriate author for the article. 11aP. in 1988, 88, 563-594; 1bP. Pico, Angio. In 2004, 43, 4412- 4456; Angio, I'm sorry. In 2004, 2004, 2004, 2004, 2004, 2004, 2017, 2017, 1cP. Schwardfgtger, M. Doleg, W.A. Schwartz, G.A. Bowmaker, P.D. Boyd, J. Physical Chemistry 1989, 91, 1762-1774; 1dH. Schwartz, Angu. 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