

## Experimental Evidence for the Formation of Fourfold Rovibrational Energy Clusters in the $\nu_1/\nu_3$ Vibrational States of $\text{H}_2^{80}\text{Se}$

J.-M. FLAUD,\* C. CAMY-PEYRET,\* H. BÜRGER,† PER JENSEN,‡  
AND IGOR N. KOZIN§

\*Laboratoire de Physique Moléculaire et Applications,<sup>1</sup> Université Pierre et Marie Curie, Bte 76, 4, Place Jussieu, F-75252 Paris Cedex 05, France; †FB 9-Anorganische Chemie and ‡FB 9-Theoretische Chemie, Bergische Universität-Gesamthochschule Wuppertal, D-42097 Wuppertal, Germany; and §Applied Physics Institute, Russian Academy of Science, Uljanov Street 46, 603 600 Nizhnii Novgorod, Russia

The present paper reports experimental evidence for the “cluster effect” (i.e., the formation of nearly degenerate, four-member groups of rotation–vibration energy levels at high rotational excitation) in the  $\nu_1/\nu_3$  vibrational states of the  $\text{H}_2^{80}\text{Se}$  molecule. The formation of such clusters in the vibrational ground state of  $\text{H}_2^{80}\text{Se}$  has been experimentally verified (see I. N. Kozin, S. Klee, P. Jensen, O. L. Polyansky, and I. M. Pavlichenkov, *J. Mol. Spectrosc.* **158**, 409–422, 1993 and references therein), K. K. Lehmann (*J. Chem. Phys.* **95**, 2361–2370, 1991) and I. N. Kozin and P. Jensen (*J. Mol. Spectrosc.* **161**, 186–207, 1993) independently predicted the existence of a new type of fourfold clusters (referred to by Kozin and Jensen as Type II clusters) in the  $\nu_1/\nu_3$  vibrational states of  $\text{H}_2^{80}\text{Se}$ . These clusters form by coalescence of two energy doublets, one belonging to the  $\nu_1$  vibrational state and one belonging to the  $\nu_3$  state. However, from the experimental data available at the time (J.-M. Flaud, C. Camy-Peyret, H. Bürger, and H. Willner, *J. Mol. Spectrosc.* **161**, 157–169, 1993) the term values of the levels predicted to form clusters could be obtained for  $J \leq 13$  only. At this  $J$  value, the term values are still far from cluster formation. For the present work, we have recorded a new FTIR spectrum of  $\text{H}_2^{80}\text{Se}$  at high pressure  $\times$  (path length) with the purpose of providing new information about the cluster formation. In this spectrum, we can follow the doublets at highest energy in the  $\nu_1$  and  $\nu_3$  states, respectively, to  $J = 18$  where the energy difference between them is  $0.94 \text{ cm}^{-1}$ . On the basis of this fact and on the basis of the trend shown by the experimentally derived term values, we conclude that the present work provides experimental verification of the formation of Type II clusters in the  $\nu_1/\nu_3$  vibrational states of  $\text{H}_2^{80}\text{Se}$ . © 1995 Academic Press, Inc.

### I. INTRODUCTION

During recent years, we have been involved in extensive experimental (1–9) and theoretical (10–12) investigations of the rotation–vibration energy level structure of  $\text{H}_2\text{Se}$ . One aim of these studies has been the characterization and possible experimental verification of the “cluster effect,” i.e., the formation of nearly degenerate, four-member groups of rotation–vibration energy levels at high rotational excitation in the rovibrational energy spectrum of this molecule. This effect, which was initially predicted by semiclassical calculations (13–16), has been experimentally verified for the vibrational ground state of  $\text{H}_2^{80}\text{Se}$  by investigations of the rotational spectrum in the submillimeter-wave and far-infrared regions (1–3). In this experimental work, the cluster structure of the rotational energy levels of the vibrational ground state could be followed for  $J \leq 23$ . The experimental results were reproduced well by purely quantum mechanical

<sup>1</sup> Laboratoire associé aux Universités Paris-Sud et P. et M. Curie.

calculations of the rotation–vibration energy level structure of  $\text{H}_2^{80}\text{Se}$  (10, 11) by means of the MORBID program system (17–19). These calculations were carried out using a potential energy function optimized to fit the lowest ( $J \leq 5$ ) rotation–vibration energy levels of  $\text{H}_2^{80}\text{Se}$  and its deuterated isotopomers (10).

The clusters in the vibrational ground state of  $\text{H}_2^{80}\text{Se}$  (referred to in Ref. (11) as Type I clusters) form by coalescence of the rotational levels with  $J_{K_a, K_c} = J_{J,0}, J_{J,1}, J_{J-1,1}$ , and  $J_{J-1,2}$  with increasing  $J$ . The theoretical calculation of Ref. (11) predicted, however, that in the  $\nu_1/\nu_3$  vibrational states of  $\text{H}_2^{80}\text{Se}$ , a qualitatively different form of cluster formation would take place in that when  $J$  increases, the  $J_{J,0}$  and  $J_{J,1}$  levels of the  $\nu_1$  vibrational state merge with the  $J_{J,0}$  and  $J_{J,1}$  levels of the  $\nu_3$  vibrational state to form a fourfold energy cluster. These clusters, which appear in manifolds of nearly degenerate vibrational states with local mode character, had previously been predicted by Lehmann (20) in model calculations. To distinguish such clusters from those observed in the vibrational ground state we refer to them as Type II clusters (11).

The energy level structure calculated for the  $\nu_1/\nu_3$  vibrational states of  $\text{H}_2^{80}\text{Se}$  in Ref. (11) agreed well with the experimentally derived term values that were available at the time (4). However, from the experimental work of Ref. (4), the  $J_{K_a, K_c} = J_{J,0}$  and  $J_{J,1}$  term values of the  $\nu_1$  and  $\nu_3$  vibrational states could be obtained for  $J \leq 13$  only. At this  $J$  value, the experimental value for the energy difference between the  $J_{K_a, K_c} = 13_{13,0}$  level of the  $\nu_1$  vibrational state and the  $13_{13,0}$  level of the  $\nu_3$  state is  $5.02 \text{ cm}^{-1}$ , so the term values are still far from cluster formation. In the present work we report the assignment of high- $K_a$  transitions in the  $\nu_1$  and  $\nu_3$  bands of  $\text{H}_2^{80}\text{Se}$  for  $J = 11$  through 18. These lines were identified in an FTIR spectrum of  $\text{H}_2^{80}\text{Se}$  recorded at high pressure  $\times$  (path length) with the purpose of providing new information about the cluster formation. With the term values determined from the positions of the new transitions we can follow the  $J_{J,0}$  and  $J_{J,1}$  levels of the  $\nu_1$  and  $\nu_3$  vibrational states up to  $J = 18$ , and the resulting energy level structure provides very strong experimental evidence for the formation of Type II clusters.

## II. EXPERIMENTAL DETAILS

The  $\text{H}_2^{80}\text{Se}$  sample was the same as used previously. Its synthesis and composition are described in Ref. (5). The sample contained  $\text{OC}^{80}\text{Se}$  and substantial quantities of  $\text{CO}_2$  which could not be removed without loss of monoisotopic  $\text{H}_2^{80}\text{Se}$ .

A high resolution spectrum was recorded at room temperature with the Bruker 120 HR interferometer at Wuppertal using a small White-type multipass cell adjusted to a path length of 6.4 m, and a total pressure of 11 mbar was chosen. The interferometer was equipped with a globar source, a KBr beam splitter, and an InSb detector. A filter eliminated radiation at wavenumbers higher than  $2950 \text{ cm}^{-1}$  and lower than  $2000 \text{ cm}^{-1}$ . The resolution (MOPD) was adjusted to  $6.5 \times 10^{-3} \text{ cm}^{-1}$ , and trapezoidal apodization was applied. A total of 1332 scans were coadded, and a signal-to-noise ratio of approximately 400 was achieved. A portion of the spectrum, with assignments given, is shown in Fig. 1.

The spectrum was calibrated with OCS lines near  $2065 \text{ cm}^{-1}$ , and the wavenumbers listed in Ref. (21) were used for this purpose. The wavenumber precision is better than  $0.5 \times 10^{-3} \text{ cm}^{-1}$ , and the wavenumber accuracy, which was checked by combination differences formed from the  $\nu_1$ ,  $\nu_1 + \nu_3$ , and  $\nu_1 + \nu_3 - \nu_1$  band systems of  $\text{OC}^{80}\text{Se}$ , is estimated to be better than  $1 \times 10^{-3} \text{ cm}^{-1}$ .

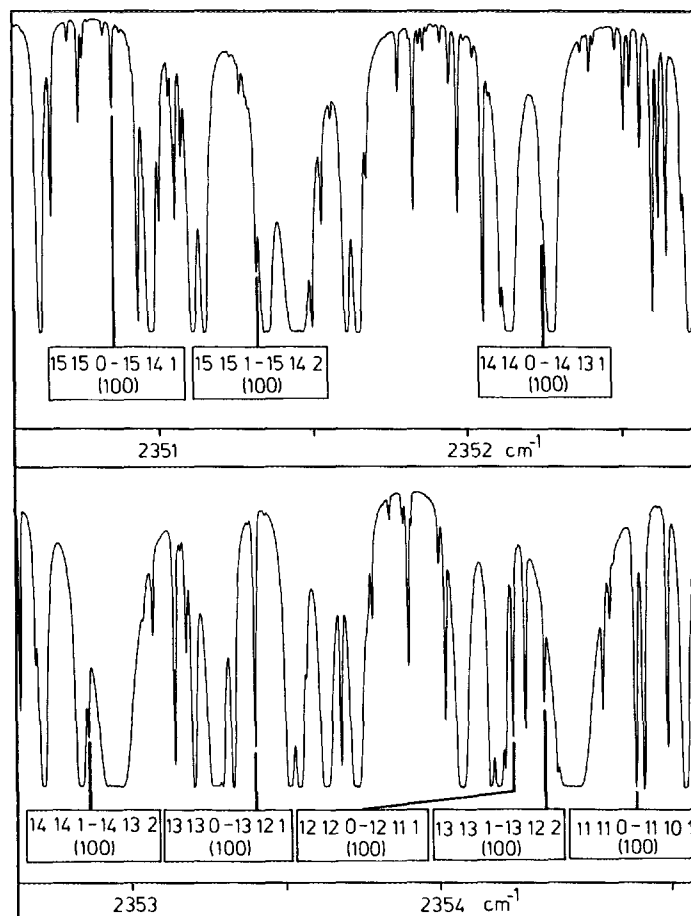


FIG. 1. A portion of the  $\text{H}_2^{80}\text{Se}$  spectrum. The assignments are indicated.

### III. ASSIGNMENT AND COMPARISON WITH THEORY

The assignments were done starting from synthetic spectra of the cold bands  $2\nu_2$ ,  $\nu_1$ , and  $\nu_3$  and of the hot bands  $\nu_1 + \nu_2 - \nu_2$  and  $\nu_2 + \nu_3 - \nu_2$  calculated with an effective, Watson-type Hamiltonian using the molecular parameters reported in Refs. (4, 7) for the upper states and those of Refs. (3, 4) for the lower states. Once a line involving a given  $K_a$  value had been assigned, the upper state constants were refined in order to provide a better extrapolation for the next  $K_a$  value. Also the intensities were checked. The final assignments are given in Table I. It should be emphasized, however, that for the highest  $K_a$  values the calculation was not sufficiently accurate for unambiguous assignments to be made. We think this is due in part to the very large mixing between the  $\nu_1$  and  $\nu_3$  basis states at high  $K_a$  and in part to convergence problems resulting from the polynomial expansion of the effective Hamiltonian.

The term values for the upper states of the transitions given in Table I are listed in Table II. They have been obtained by combining the transition wavenumbers of Table I with term values for the rotational levels in the vibrational ground state of  $\text{H}_2^{80}\text{Se}$ . These latter term values were calculated with the effective Hamiltonian of Ref. (4)

TABLE I  
Experimentally Determined Line Positions (in cm<sup>-1</sup>) in the  $\nu_1$  and  $\nu_3$  Bands of H<sub>2</sub><sup>80</sup>Se

$\nu_1$ band							$\nu_3$ band						
$J'$	$K'_a$	$K'_c$	$J''$	$K''_a$	$K''_c$	$\nu_{\text{obs}}$	$J'$	$K'_a$	$K'_c$	$J''$	$K''_a$	$K''_c$	$\nu_{\text{obs}}$
11	11	0	11	10	1	2354.665	11	11	0	11	11	1	2342.309
11	11	1	11	10	2	2356.742	11	11	1	11	11	0	2341.885
12	12	0	12	11	1	2354.238	12	12	0	12	12	1	2339.961
12	12	1	12	11	2	2355.641	12	12	1	12	12	0	2339.662
13	13	0	13	12	1	2353.404	13	13	0	13	13	1	2337.743
13	13	1	13	12	2	2354.340	13	13	1	13	13	0	2337.528
14	14	0	14	13	1	2352.243	14	14	0	14	14	1	2335.768
14	14	1	14	13	2	2352.865	14	14	1	14	14	0	2335.607
15	15	0	15	14	1	2350.852							
15	15	1	15	14	2	2351.265	15	15	1	15	15	0	2334.034
16	16	1	16	15	2	2349.612	16	16	0	16	16	1	2333.022
17	17	0	17	16	1	2347.792 <sup>a</sup>							
17	17	1	17	16	2	2347.981	17	17	0	17	17	1	2332.473
18	18	1	18	17	2	2346.466 <sup>b</sup>	18	18	0	18	18	1	2332.546 <sup>c</sup>

<sup>a</sup>Calculated as the average of the wavenumbers of two possible candidates for this assignment, a blended line at 2347.800 cm<sup>-1</sup> and a line at 2347.783 cm<sup>-1</sup>.

<sup>b</sup>Blended line.

<sup>c</sup>Calculated as the average of the wavenumbers of three possible candidates for this assignment, a strong line at 2332.553 cm<sup>-1</sup>, a blended line at 2332.564 cm<sup>-1</sup>, and a line at 2332.522 cm<sup>-1</sup>.

using the parameters of Refs. (3, 4). Table II gives also the energy difference  $\Delta E$  between the state in question and the highest possible energy at the given  $J$  value (which belongs to the  $\nu_3$  level with  $J_{K_a, K_c} = J_{J,0}$ ) when this energy is available.

The experimentally derived term values of Table II have been used together with those in Table III of Ref. (4) to generate a set of energy differences for the rotational states in the  $\nu_1$ ,  $\nu_3$ , and  $2\nu_2$  vibrational states. For the multiplet of rotational levels belonging to these three vibrational states, we calculate for each  $J$  value the term values relative to the highest rotation-vibration energy possible for that particular  $J$ . These energy differences are included in Fig. 2, which shows an overview of the rotation-vibration term values for H<sub>2</sub><sup>80</sup>Se in the  $\nu_1/\nu_3/2\nu_2$  region for  $J \leq 35$ . As mentioned above, the term values are plotted relative to the highest energy for each  $J$  multiplet. The three states present for  $J = 0$  are the  $\nu_3$  (at 2358 cm<sup>-1</sup>),  $\nu_1$  (at 2344 cm<sup>-1</sup>), and  $2\nu_2$  (at 2060 cm<sup>-1</sup>) levels. The term values calculated by the MORBID program (using the parameters from Table II of Ref. (10)) are given as horizontal lines, and experimentally derived term values are shown as circles. Filled circles represent term values that were included in the input data for the MORBID fitting of Ref. (10) ( $J \leq 5$ ); empty circles represent experimental term values which were not included.

TABLE II  
Experimentally Derived Term Values (in  $\text{cm}^{-1}$ ) in the  $\nu_1$  and  $\nu_3$   
Vibrational States of  $\text{H}_2^{80}\text{Se}$

$\nu_1$ state					$\nu_3$ state				
$J$	$K_a$	$K_c$	$E$	$\Delta E^a$	$J$	$K_a$	$K_c$	$E$	$\Delta E^a$
11	11	1	3383.714	-6.794	11	11	1	3390.251	-0.257
11	11	0	3383.448	-7.060	11	11	0	3390.508	
12	12	1	3570.732	-5.861	12	12	1	3576.410	-0.183
12	12	0	3570.546	-6.047	12	12	0	3576.593	
13	13	1	3772.610	-4.883	13	13	1	3777.360	-0.133
13	13	0	3772.478	-5.015	13	13	0	3777.493	
14	14	1	3989.206	-3.906	14	14	1	3993.011	-0.101
14	14	0	3989.111	-4.001	14	14	0	3993.112	
15	15	1	4220.393		15	15	1	4223.293	
15	15	0	4220.323						
16	16	1	4466.060	-2.141	16	16	0	4468.201	
17	17	1	4726.107	-1.457					
17	17	0	4726.064	-1.500	17	17	0	4727.564	
18	18	1	5000.451	-0.937	18	18	0	5001.388	

$$^a \Delta E = E - E(\nu_3, J_{K_a, K_c} = J_{J,0}).$$

For greater clarity, we show in Fig. 3a an enlargement of the upper  $50 \text{ cm}^{-1}$  of Fig. 2. Figure 3b shows, on the same enlarged scale, the experimentally derived term values only. The vibrational assignment of each energy level, as obtained from the experimental spectrum, is indicated.

#### IV. DISCUSSION

The quantities  $\Delta E$  of Table II measure the energy distances between molecular states which, according to the theoretical predictions of Ref. (11), will merge in the limit of  $J \rightarrow \infty$  to form a fourfold cluster. We see that the  $\Delta E$  values decrease with increasing  $J$ , thus confirming that clusters are formed. As mentioned above, the experimental value for the energy difference between the  $J_{K_a, K_c} = 13_{13,0}$  level of the  $\nu_1$  vibrational state and the  $13_{13,0}$  level of the  $\nu_3$  state is  $5.02 \text{ cm}^{-1}$ , but the analogous difference at  $J = 18$  between the  $18_{18,1}$  level of the  $\nu_1$  vibrational state and the  $18_{18,0}$  level of the  $\nu_3$  state has decreased to  $0.94 \text{ cm}^{-1}$ . The cluster formation is illustrated more clearly by Fig. 2. On the scale of this figure, there appears to be close agreement between the results of the MORBID calculation and the experimentally derived term values. The enlargement in Fig. 3a reveals that the distances between cluster states calculated by MORBID are systematically smaller than the experimentally derived values. However, the qualitative trend exhibited by the experimentally derived term values closely follows that suggested by the MORBID calculation; the two energy doublets at highest energy in the figure merge to form fourfold clusters as  $J$  increases.

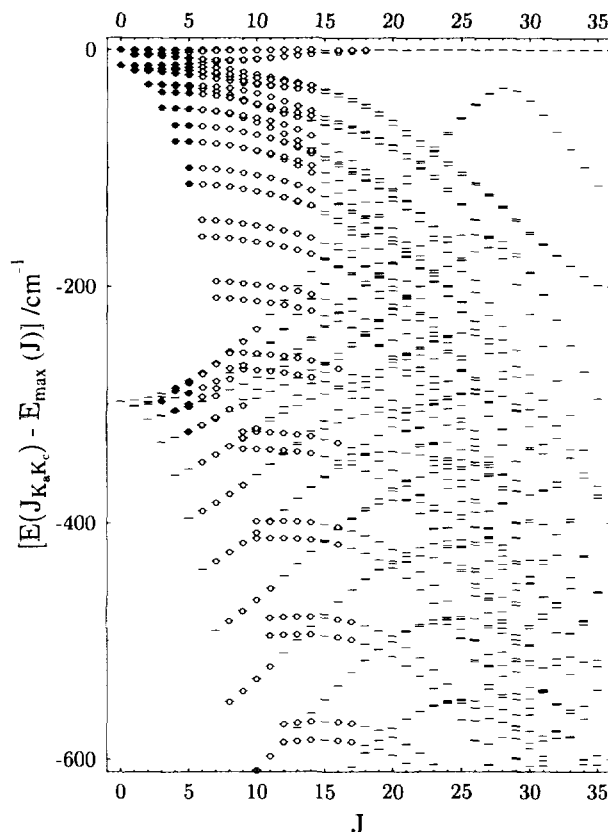


FIG. 2. An overview of the rotation-vibration term values for  $\text{H}_2^{80}\text{Se}$  in the  $\nu_1/\nu_3/2\nu_2$  region. The term values are plotted relative to the highest energy for each  $J$  multiplet. The three states present for  $J = 0$  are the  $\nu_3$  (at  $2358\text{ cm}^{-1}$ ),  $\nu_1$  (at  $2344\text{ cm}^{-1}$ ), and  $2\nu_2$  (at  $2060\text{ cm}^{-1}$ ) levels. The term values calculated by the MORBID program (using the parameters from Table II of Ref. (10)) are given as horizontal lines, and experimentally derived term values are shown as circles. Filled circles represent term values that were included in the input data for the MORBID fitting of Ref. (10) ( $J \leq 5$ ); empty circles represent experimental term values which were not included.

Figure 3b illustrates that the clusters are formed by coalescence of two doublets belonging to different vibrational states. The doublet at highest energy belongs to the  $\nu_3$  vibrational state, and it merges with a doublet belonging to the  $\nu_1$  vibrational state. As discussed in detail in Ref. (11), the resulting cluster states are 50–50 mixtures of  $\nu_1$  and  $\nu_3$  vibrational basis states, and this leads to a very interesting stretching motion in these cluster states.

In the variational MORBID calculation, the cluster formation is the result of very subtle mechanisms involving, in the case of the Type II clusters discussed here, predominantly the Coriolis-type interaction between the  $\nu_1$  and  $\nu_3$  basis states but also interactions with other vibrational basis states responsible for the centrifugal distortion effects from the bending motion. Consequently, it is difficult to understand why the MORBID calculation of Ref. (11) yields distances between cluster states that are systematically smaller than those determined experimentally (Fig. 3a). One conceivable reason could be that in the MORBID fitting (10) which produced the potential energy function used in Ref. (11), the residual (obs. – calc.) for the  $\nu_1$   $J_{K_a, K_c} = 0_{0,0}$  energy is  $-0.009\text{ cm}^{-1}$ , whereas that for the  $\nu_3$   $J_{K_a, K_c} = 0_{0,0}$  energy is  $+0.066\text{ cm}^{-1}$  (Table I of

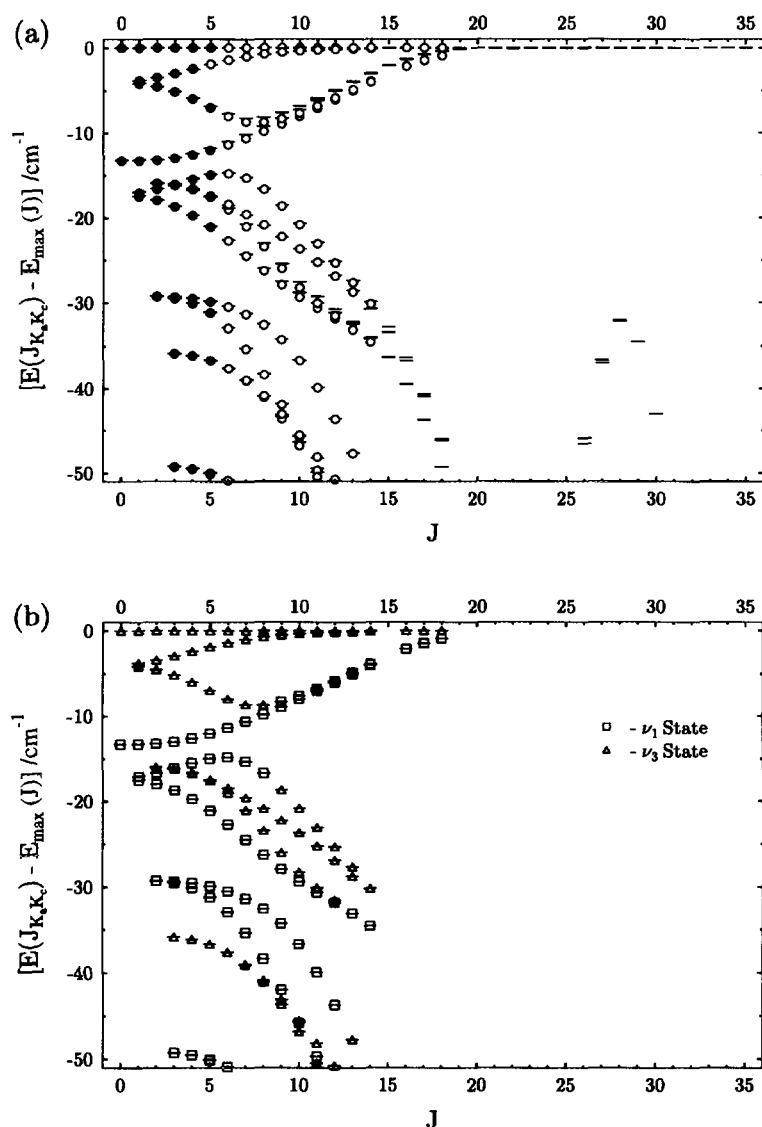


FIG. 3. (a) An enlargement of the upper  $50 \text{ cm}^{-1}$  of Fig. 2 showing term values of  $\text{H}_2^{80}\text{Se}$  in the  $\nu_1/\nu_3/2\nu_2$  region. Term values calculated by the MORBID program (using the parameters from Table II of Ref. (10)) are given as horizontal lines, and experimentally derived term values are shown as circles. Filled circles represent term values that were included in the input data for the MORBID fitting of Ref. (10) ( $J \leq 5$ ); empty circles represent experimental term values which were not included. (b) The experimentally derived term values. The vibrational assignment of each energy level, as obtained from the experimental spectrum, is indicated.

Ref. (10)). Since the  $\nu_3$  vibrational energy is higher than the  $\nu_1$  energy, this means that the energy difference between the two  $J = 0$  energies is calculated to be too small by  $0.075 \text{ cm}^{-1}$ . This leads to a systematic reduction of the energy differences between the interacting  $\nu_1$  and  $\nu_3$  basis states, which at higher  $J$  values participate in the cluster formation. This in turn increases the mixing of these states which may accelerate the

formation of clusters. The potential surface used for the MORBID calculations of Ref. (11) was obtained by fitting to rotation-vibration energy spacings involving  $J \leq 5$ . We plan a fitting to data involving higher  $J$  values; the resulting potential energy function may provide better agreement with experiment for the cluster splittings.

Inspection of Table II shows that during the cluster formation, the sequence of energy levels deviates from that expected for an asymmetric rotor. In the  $\nu_1$  vibrational state, the  $J_{K_a, K_c} = J_{J,0}$  state (which has  $A_1$  symmetry for  $J$  even and  $B_2$  symmetry for  $J$  odd; we label the irreducible representations of the molecular symmetry group as given in Table A-4 of Ref. (22)) is systematically lower in energy than the  $J_{J,1}$  state (which has  $B_1$  symmetry for  $J$  even and  $A_2$  symmetry for  $J$  odd). This trend starts at  $J = 9$  (see Table III of Ref. (4)) and is reproduced by the MORBID calculation of Ref. (11).

For each of the  $J$  values 16 and 18, only two transitions to the  $\nu_1/\nu_3$  cluster states have been observed. For  $J = 17$ , three such transitions have been observed. However, we know that the cluster forms by coalescence of two nearly degenerate doublets; a  $\nu_1$  doublet (consisting of two states spanning the reducible representation  $A_1 + B_1$  of  $C_{2v}$  for  $J$  even and  $A_2 + B_2$  for  $J$  odd) and a  $\nu_3$  doublet (consisting of two states spanning the reducible representation  $A_2 + B_2$  for  $J$  even and  $A_1 + B_1$  for  $J$  odd). The trends shown by the experimentally derived term values in Table II and in Table III of Ref. (4), the calculations of Lehmann (20), and the MORBID predictions (10, 11) provide evidence for this behavior. In the semiclassical picture (see, for example, Refs. (10, 11) and references therein) the doublet states are equivalent in that one doublet state is obtained from the other by inversion of the angular momentum vector  $\mathbf{J}$ . The transitions measured for each  $\nu_1/\nu_3$  cluster in the  $J$  range from 16 through 18 define at least one term value in each coalescing doublet. Hence these transitions give a good estimation of the total cluster "size."

As mentioned in Section I, the formation of Type I clusters in the vibrational ground state of  $\text{H}_2^{80}\text{Se}$  has been experimentally verified in Refs. (1-3). The arguments put in favor of this cluster formation are mainly in the form of term value diagrams derived from experiment such as Fig. 4 of Ref. (1) and Fig. 2 of Ref. (10). At present, the relevant rotational term values in the vibrational ground state of  $\text{H}_2^{80}\text{Se}$  can be followed up to  $J = 23$  (see Fig. 2 of Ref. (10)), where the experimentally derived energy difference between the two doublets at highest energy is  $3.95 \text{ cm}^{-1}$ . In the present work, we follow the doublets at highest energy in the  $\nu_1$  and  $\nu_3$  states, respectively, to  $J = 18$  where the energy difference between them is  $0.94 \text{ cm}^{-1}$ . On the basis of this fact and on the basis of the trend shown by the experimentally derived term values in Figs. 2 and 3, we conclude that the present work provides experimental verification of the formation of Type II clusters in the  $\nu_1/\nu_3$  vibrational states of  $\text{H}_2^{80}\text{Se}$ .

#### ACKNOWLEDGMENTS

We thank P. R. Bunker for critically reading the manuscript and suggesting improvements. This work was supported by the Deutsche Forschungsgemeinschaft (through Forschergruppe Grant Bu 152/12-3) and by the Fonds der Chemischen Industrie. I.N.K. thanks the Russian Fund for Fundamental Investigations (Grant N94-02-05424-a), the International Science Foundation (Grant R81000), and M. Yu. Tretyakov.

RECEIVED: December 29, 1994

#### REFERENCES

1. I. N. KOZIN, S. P. BELOV, O. L. POLYANSKY, AND M. YU. TRETYAKOV, *J. Mol. Spectrosc.* **152**, 13-28 (1992).



2. I. N. KOZIN, O. L. POLYANSKY, S. I. PRIPOLZIN, AND V. L. VAKS, *J. Mol. Spectrosc.* **156**, 504–506 (1992).
3. I. N. KOZIN, S. KLEE, P. JENSEN, O. L. POLYANSKY, AND I. M. PAVLICHENKOV, *J. Mol. Spectrosc.* **158**, 409–422 (1993).
4. J.-M. FLAUD, C. CAMY-PEYRET, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **161**, 157–169 (1993).
5. J.-M. FLAUD, C. CAMY-PEYRET, P. ARCAS, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **165**, 124–136 (1994).
6. J.-M. FLAUD, P. ARCAS, C. CAMY-PEYRET, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **166**, 204–209 (1994).
7. J.-M. FLAUD, C. CAMY-PEYRET, P. ARCAS, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **167**, 383–399 (1994).
8. J.-M. FLAUD, C. CAMY-PEYRET, P. ARCAS, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **168**, 556–566 (1994).
9. J.-M. FLAUD, P. ARCAS, C. CAMY-PEYRET, H. BÜRGER, AND H. WILLNER, *J. Mol. Spectrosc.* **170**, 534–541 (1995).
10. P. JENSEN AND I. N. KOZIN, *J. Mol. Spectrosc.* **160**, 39–57 (1993).
11. I. N. KOZIN AND P. JENSEN, *J. Mol. Spectrosc.* **161**, 186–207 (1993).
12. P. JENSEN AND P. R. BUNKER, *J. Mol. Spectrosc.* **164**, 315–317 (1994).
13. B. I. ZHILINSKII AND I. M. PAVLICHENKOV, *Opt. Spectrosc. (USSR)* **64**, 688–690 (1988). [In Russian]
14. J. MAKAREWICZ AND J. PYKA, *Mol. Phys.* **68**, 107–127 (1989).
15. J. MAKAREWICZ, *Mol. Phys.* **69**, 903–921 (1990).
16. J. PYKA, *Mol. Phys.* **70**, 547–561 (1990).
17. P. JENSEN, *J. Mol. Spectrosc.* **128**, 478–501 (1988).
18. P. JENSEN, *J. Chem. Soc. Faraday Trans. 2* **84**, 1315–1340 (1988).
19. P. JENSEN, in “Methods in Computational Molecular Physics” (S. Wilson and G. H. F. Diercksen, Eds.), Plenum, New York, 1992.
20. K. K. LEHMANN, *J. Chem. Phys.* **95**, 2361–2370 (1991).
21. A. G. MAKI AND J. S. WELLS, “Wavenumber Calibration Tables from Heterodyne Frequency Measurements,” NIST Special Publication 821, Washington, DC, 1991.
22. P. R. BUNKER, “Molecular Symmetry and Spectroscopy,” Academic Press, New York, 1979.