Bushes of normal modes for nonlinear mechanical systems with discrete symmetry

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Abstract
The normal modes in a linear mechanical system with discrete symmetry are independent of each other. When such systems are non-linear, these modes are all coupled to each other. However, if a single mode is excited, this excitation spreads to only a finite number of other modes. This collection of modes is called a "bush of modes". The dynamical behavior of a bush of modes depends on the form of its Hamiltonian. This allows us to put bushes into universality classes. As an example, we list the one, two, and three-dimensional bushes for all possible free molecules with crystallographic point-group symmetry. (Our analysis can be applied not only to molecules but to any macroscopic mechanical system with point symmetry as well.) We find 363 distinct bushes that belong to 11 different classes. We give the form of the Hamiltonian for each of those 11 classes.

1 Introduction

Investigation of nonlinear oscillations in dynamical systems with discrete symmetries is an important research direction in nonlinear mechanics. Three-dimensional mechanical objects with point symmetry and one-dimensional chains with translational symmetry are examples of such dynamical systems. Crystals described by one of 230 space groups are more complicated but are also typical physical objects with discrete symmetry. Group-theoretical methods are a powerful tool for the investigation of complex nonlinear systems with various types of symmetry. The Lie group analysis of differential equations for systems with continuous symmetries is well developed and very intensively exploited. However, group-theoretical methods for nonlinear dynamical systems characterized by discrete symmetry groups are rather seldomly employed.

The new concept "bushes of normal modes" for physical systems with discrete symmetry was introduced by us in [1]. This concept seems to be as fundamental as the concepts of solitons, dissipative structures, etc. in modern nonlinear science.

A given bush is a certain set of primary and secondary modes closed under their interactive forces. Excitation of a primary ("root") mode leads to the excitation of the bush as a single dynamical object. The amplitudes of modes belonging to the bush change in time and, as a rule, their evolution is not trivial. As a consequence, we can speak about a number of new types of excitations in systems with discrete symmetry.

In the above mentioned paper [1] and in [2, 3] we investigated the main properties of bushes of modes and developed the general group-theoretical method for finding them.

The detailed discussion of our approach and some important theorems as well as possible physical applications were presented in [4]. Bushes of small dimensionality for many structures with point and space groups of crystallographic symmetry were found, classified, and investigated in the above papers. Since the application of group-theoretical methods in finding bushes of modes for mechanical systems described by space groups with multidimensional irreducible representations (irreps) is very difficult, we developed appropriate computer software for treating such problems. (Previously similar programs were used for studying structural phase transitions in crystals [5, 6].)

New possibilities for studying bush problems in complex mechanical structures appeared due to the collaboration of the Rostov (Russia) research group headed by Sakhnenko and Chechin and the Provo (USA) research group headed by Hatch and Stokes. During the two previous decades our groups independently developed group-theoretical methods for studying phase transitions in crystals (see [7, 8, 5, 9, 10, 11] and the papers cited therein). The powerful computer program ISOTROPY, which utilizes a great number of group theoretical methods used in the theory of crystals, was created by the Provo group. This program, including the ability to treat bushes of normal modes is available on Internet as free software [12].

The paper [13] devoted to nonlinear normal modes in the systems with discrete symmetry was published as a result of the above mentioned collaboration. All "irreducible" bushes of vibrational modes for all mechanical systems with the symmetry of any of the 230 space groups was found in this paper. These bushes were classified into 19 classes of dynamical universality for the case of analytical potentials. For all possible crystals, we obtained all symmetry-determined similar nonlinear normal modes, introduced in [14] by Rosenberg, and all resonance subspaces used in studying the stability of nonlinear normal modes (see papers [15, 16, 17] by Montaldi, Roberts and Stewart). It is interesting that there exists no *symmetry-determined* resonance subspaces whose dimensionality exceed four.

The recently published paper [18] by Poggi and Ruffo is devoted to the dynamics of the Fermi-Pasta-Ulam chain of β-type. These authors revealed some exact solutions for the considered mechanical system and demonstrated "the existence of subsets of normal modes where energy remains trapped for suitable initial conditions", which they called "subsets of I-type".

Note:

- The analysis in [18] is based on the specific character of interaction between particles of the FPU-β chain and, therefore, such an analysis must be done once again for every other different monatomic chain.
- Only one- and two-dimensional subsets of normal modes of "type I" were found for FPU-β in [18].

The dynamical objects discussed by Poggi and Ruffo prove to be a very special case of bushes of normal modes for one-dimensional monatomic chains with periodic boundary conditions. They can be easily obtained by our general group-theoretical method for treating bushes of vibrational modes in three-dimensional mechanical systems with any space symmetry [19].

The outline of the approach to studying nonlinear dynamics of the systems with discrete symmetry based on the concept of bushes of normal modes is presented in the first part of this paper. The list of low-dimensional bushes of vibrational modes for *all* N-particle mechanical systems with any of the 32 point groups of crystallographic symmetry is given in the second part of the paper.

2 Two types of mode interactions

We consider the classical Hamiltonian systems of N particles moving near the single equilibrium state with the space or point group G_0. Let the Cartesian coordinates x_i ($i = 1, \ldots, 3N$), characterizing the deviations of every particle (along the X, Y, Z axes) from its equilibrium position, and the momenta $p_i = m_i\dot{x}_i$ ($i = 1, \ldots, 3N$) corresponding to them, be the initial dynamical variables. A reducible representation Γ of the group G_0 which is realized in the 3N-dimensional configuration space S of the system is called the mechanical representation. It can be decomposed into a number of subspaces, invariant with respect to the group G_0, by means of a suitable linear transformation. Evidently, the set x_i ($i = 1, \ldots, 3N$) and the set $p_i = m_i\dot{x}_i$ ($i = 1, \ldots, 3N$) are transformed under the action of any element $g \in G_0$ independently and identically. Therefore, the momentum space is decomposed into the invariant subspaces in just the same manner as the configurational one (regarding the number of the subspaces of each given type).

Let S_j ($j = 1, 2, \ldots$) be invariant subspaces of the smallest dimensions (n_j) and $\varphi_j^{(i)}$ ($i = 1, 2, \ldots, n_j$) be a basis of S_j. It is well-known that irreducible representations Γ_j of group G_0 are realized in subspaces S_j, and $\boldsymbol{\varphi}_j^{(i)}$ ($i = 1, 2, \ldots, n_j$) are often called basis vectors of these irreps. The complete set of basis vectors of all irreps entering into decomposition of the mechanical representation Γ forms a basis of the 3N-dimensional configuration space S. Therefore we can write an arbitrary vector $\mathbf{x}(t) \in S$, which determines the system configuration at the moment t, as a superposition of basis vectors $\boldsymbol{\varphi}_{\boldsymbol{j}}^{\boldsymbol{(i)}}$ of all irreps Γ_j of group G_0:

$$\mathbf{x}(t) = \sum_{j,i} \mu_j^{(i)}(t)\boldsymbol{\varphi}_j^{(i)} \tag{1}$$

The complete set of $3N$ coefficients $\mu_j^{(i)}$ of this superposition is a set of new dynamical variables instead of the old variables x_i ($i = 1, \ldots, 3N$). An action of $g \in G_0$ on the space variable $\mathbf{r}$, which is an argument of basis vectors $\boldsymbol{\varphi}_j^{(i)}$ ($i = 1, 2, \ldots, n_j$) of irrep Γ_j, induces an action of matrix $M_j(g) \in \Gamma_j$ on variables $\boldsymbol{\mu}_j(t) = \{\mu_j^{(i)}(t) | i = 1, 2, \ldots, n_j\}$. It is in this sense that we shall say hereafter that (1) variables $\mu_j^{(i)}(t)$ ($i = 1, 2, \ldots, n_j$) are transformed according to the irrep Γ_j, or (2) $\boldsymbol{\mu}_j(t)$ correspond to Γ_j, or (3) $\boldsymbol{\mu}_j(t)$ are associated with the irrep Γ_j. All three of these expressions will be used in the present paper as synonymous. It is convenient to consider the complete set of n_j variables $\mu_j^{(i)}(t)$ ($i = 1, 2, \ldots, n_j$) as a n_j-dimensional vector and refer to it as to the vector variable $\boldsymbol{\mu}_j(t) = (\mu_j^{(1)}(t), \ldots, \mu_j^{(n_j)}(t))$ associated with the irrep Γ_j. Sometimes, variables $\mu_j^{(i)}$ will be named symmetry-adapted modes, or simply, modes. (In a particular case they can be normal modes.)

The decomposition of the configuration space into invariant subspaces is a purely geometric procedure, but it plays an important role in the dynamical studies. Indeed, the variables corresponding to different irreps of group G_0 are independent of each other in the harmonic approximation. The Hamiltonian in such an approximation will be denoted by H_2. The transition to basis vectors of the irreps of group G_0 leads to the simplest form of H_2 provided that only one-dimensional irreps with the unity multiplicity enter into the configuration representation. In other cases the normal coordinates (normal modes) may be introduced in the standard manner. They are classified by the irreps of group G_0 and are independent in the harmonic approximation.

However, the excitation of a given normal mode generally leads to the excitation of a number of other normal modes, associated with the different irreps Γ_j, if *anharmonic interactions* between modes are taken into account. The symmetry-related selection rules regulating the excitation transfer from a certain mode to modes of a quite definite set of irreps Γ_j were found in [1]. The dynamical nature of these selection rules is connected with the existence of two types of mode interactions, which we called the "force" and the "parametric" type. Let us explain the difference between these types of interactions with the aid of a simple system of two coupled linear oscillators whose interaction energy is described by only one anharmonic term $U = -\gamma x_1^2 x_2$. The equations of motion for such a system are

$$\ddot{x}_1 + \omega_1^2 x_1 = 2\gamma x_1 x_2 \tag{2}$$

$$\ddot{x}_2 + \omega_2^2 x_2 = \gamma x_1^2 \tag{3}$$

The disparity of the modes $x_1(t)$ and $x_2(t)$ can be readily revealed from the specific structure of these equations. Indeed, the excitation of the mode $x_1(t)$ leads necessarily to the appearance of the mode $x_2(t)$, even if the latter was not excited at the initial moment, since Eq.(3) does not permit the solution $x_1(t) \not\equiv 0, x_2(t) \equiv 0$. Using physical arguments, one may say that the excitation of $x_1(t)$ gives rise to the appearance of the force $\left(-\frac{\partial U}{\partial x_2} = \gamma x_1^2\right)$ in the right-hand side of Eq.(3) for mode $x_2(t)$, and in this sense we shall speak of a "force" action exerted by mode $x_1(t)$ on mode $x_2(t)$.

On the other hand, Eqs.(2,3) possess the solution $x_1(t) \equiv 0, x_2(t) \not\equiv 0$ and therefore the excitation of the mode $x_2(t)$ does not lead, in general, to the excitation of the mode $x_1(t)$. In other words, the right-hand side of Eq.(2) equals zero when $x_1(t) \equiv 0$, and mode $x_2(t)$ does not exert any force on $x_1(t)$ in such a case. Nevertheless, mode $x_1(t)$ could still become excited in this system because of the phenomenon similar to parametric resonance. Indeed, Eq.(3) becomes that of the harmonic oscillator when $x_1(t) \equiv 0$, and its general solution is $x_2(t) = A\cos(\omega_2 t + \delta)$. The substitution of this solution into Eq.(2) reduces it, after some manipulations, to the well-known Mathieu equation. According to the Floquet theory, there exist coefficient domains of the Mathieu equation, which correspond to stable and unstable solutions. It is in the latter domains that the parametric excitation of mode $x_1(t)$ takes place.

The above-considered cases exhibit the fundamental distinction between mode interactions of the two types, i.e., the force and the parametric interactions. This difference exists in the most general case as well [1]. We wish to stress once more that the interaction which was called parametric actually leads to the parametric excitation of a certain mode only in the domain of unstable mechanical motion. However, as follows from simple estimations, for most problems of nonlinear dynamics of molecules and crystal lattices the above-mentioned parametric instability does not occur in view of the numerical values of the pertinent physical parameters. It means that in a typical situation the system's motion is stable and, therefore, new modes are excited because of the force interactions only. Moreover, when a certain dynamical regime loses its stability, the nonlinear system usually enters a new regime with the main role again being played by the force interactions between the modes.

3 Bushes of modes for a dynamical system

Now let us consider the interactions between the modes of an arbitrary N-particle nonlinear Hamiltonian system with discrete symmetry group G_0 in its equilibrium state. The potential function of this system is invariant with respect to all the elements $g \in G_0$. Starting with $3N$ Cartesian coordinates of individual particles we can go over to the $3N$ normal modes $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_{3N})$ satisfying the dynamical equations of the Newton type (this point is considered in detail in [4]):

$$\ddot{\mu}_i = -\frac{\partial V}{\partial \mu_i}, \quad i = 1, \ldots, 3N. \tag{4}$$

Here the potential energy $V(\boldsymbol{\mu})$ remains invariant under the action of all matrices of the mechanical representation Γ of the system in hand. Assuming $V(\boldsymbol{\mu})$ to be an analytical function, we can write it as a superposition of all possible polynomial invariants of the representation Γ.

Let Γ_ξ and Γ_η be two irreps contained in the decomposition of the reducible representation Γ into its irreducible parts, and let $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$ and $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots)$ be two vectorial variables which are transformed according to Γ_ξ and Γ_η, respectively. We can reveal the condition under which the excitation of one of these variables $(\boldsymbol{\xi})$ necessarily leads to the excitation of the other $(\boldsymbol{\eta})$. We have already discussed the difference between the "force" and "parametric" interactions using the simple example (2,3). In general, one can speak of the force or parametric action of the variable $\boldsymbol{\xi}$ upon the variable $\boldsymbol{\eta}$ in accordance with the structure of mixed invariants constructed from their components. Let us consider a mixed invariant $L_{k,p}$ which is a homogeneous function of the kth power in the components of $\boldsymbol{\xi}$ and the pth power in the components of $\boldsymbol{\eta}$. There is a fundamental distinction in the structure of the equations (4) for the cases $p = 1$ and $p > 1$.

First, let us study the case $p = 1$, where there exists a mixed invariant,

$$L_{k,1} = \sum_i \eta_i f_i^{(k)}(\boldsymbol{\xi}), \tag{5}$$

where $f_i^{(k)}(\boldsymbol{\xi})$ are the polynomials of the kth power with respect to the components of $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$. In this case certain terms independent of the variable $\boldsymbol{\eta}$, induced by the invariant (5), will be contained in the right-hand sides of the dynamical equations (4) corresponding to the components of $\boldsymbol{\eta}$:

$$\ddot{\eta}_i = -\frac{\partial V}{\partial \eta_i} = -f_i^{(k)}(\boldsymbol{\xi}) + \cdots, \quad (i = 1, 2, \ldots). \tag{6}$$

These right-hand sides, which may be treated as forces, are not equal to zero when $\boldsymbol{\xi}(t) \not\equiv 0$ at least for one or more values of i. Indeed, the assumption that $\boldsymbol{\eta}(t) \equiv 0$ when $\boldsymbol{\xi}(t) \not\equiv 0$ leads to a contradiction with respect to the specific structure of (6). Therefore, in the case of $p = 1$, some components of $\boldsymbol{\eta}$ get excited because of the force acting from $\boldsymbol{\xi}$ on $\boldsymbol{\eta}$.

Now let us examine the case when the group of symmetry G_0 permits the existence of the invariants $L_{k,p}$ with $p > 1$ only. Then the right-hand side of each equation of the system (4) is proportional to some positive power of components of the variable $\boldsymbol{\eta}$ and, therefore, there exists a solution with $\boldsymbol{\eta}(t) \equiv 0$ in spite of $\boldsymbol{\xi}(t) \not\equiv 0$. In other words, $\boldsymbol{\eta}$ continues to be zero at all times if it was not excited at the initial moment. Namely in this sense we say that $\boldsymbol{\xi}$ does not excite $\boldsymbol{\eta}$. Thus, the force action of $\boldsymbol{\xi}$ on the initially non-excited variable $\boldsymbol{\eta}$ takes place if and only if the symmetry allows the existence of the mixed invariants $L_{k,1}$, linear in the components of the variable $\boldsymbol{\eta}$. Some additional clarification at this point is in order. It is clear from the discussion concerning equations (2,3) that even in the absence of the invariants $L_{k,1}$ the variable $\boldsymbol{\eta}$ may sometimes spontaneously arise because of a phenomenon similar to the parametric resonance. Such an appearance of $\boldsymbol{\eta}$ can be possible only in the domains of unstable motion, and these domains depend both on the parameters of the given physical system and on initial conditions. As soon as the variable $\boldsymbol{\eta}$ has arisen, force action on it from the variable $\boldsymbol{\xi}$ occurs, and thereby the set of variables coupled by this force action is enlarged.

Because of the great significance of the $L_{k,1}$-type invariants in classical dynamics, it is desirable to find a suitable criterion of their existence. It is well known (see, e.g., [20]) that the invariants $L_{k,1}$ exist if and only if the irrep Γ_η is contained in a certain direct power of irrep Γ_ξ. We proposed in [4] a more convenient criterion based on the group-subgroup relation between the kernels of these two irreps. It underlies a method, much simpler than all known methods, for singling out the complete set of dynamical variables, connected with each other by the force action. Indeed, this rather difficult problem can be solved by a one-step geometrical procedure as contrasted to the complicated analysis of the sequential direct powers of the irreps of group G_0.

Let us introduce the following notations. $\Gamma_j^{\otimes k} \equiv \underbrace{\Gamma_j \otimes \Gamma_j \otimes \ldots \otimes \Gamma_j}_{k\ times}$ is the kth direct (Kronecker) power of irrep Γ_j of group G_0. $Ker\Gamma_j$ is the kernel of homomorphism of the irrep Γ_j, i.e., the set of all elements $g \in G_0$ which corresponds to the identity matrix in this representation. The relation $\Gamma_j \in \Gamma_j^{\otimes k}$ means that Γ_j is contained in the decomposition of the reducible representation $\Gamma_j^{\otimes k}$ into irreducible representations of group G_0. The following theorem was proved in [4].

Theorem.

Let Γ_ξ and Γ_η be two irreps of group G_0. Then $\Gamma_\eta \in \Gamma_\xi^{\otimes k}$ will be true for some positive integer k, if and only if $Ker\Gamma_\xi \leq Ker\Gamma_\eta$. In the case that $Ker\Gamma_\xi \leq Ker\Gamma_\eta$, the smallest value of k for which $\Gamma_\eta \in \Gamma_\xi^{\otimes k}$ is true has an upper bound M (i.e., $k \leq M$) which is given by the number M of the distinct nonzero values of the traces $\chi_\xi(g), g \in G_0$, of the matrices of the irrep Γ_ξ.

In a certain sense, $Ker\Gamma_\xi$ may be treated as a group of symmetry associated with the variable $\boldsymbol{\xi}$, which makes it possible to refer to $Ker\Gamma_\xi$ as the ker-symmetry of this variable. Based on the above Theorem we may state that the variable $\boldsymbol{\xi}$ excites the variable $\boldsymbol{\eta}$ if and only if the ker-symmetry of $\boldsymbol{\xi}$ is less than or equal to that of $\boldsymbol{\eta}$.

The dynamical variable $\boldsymbol{\xi}(t)$ initially excited in the system will be called the *root* or *primary* variable. Its appearance leads to the excitation of a number of secondary variables. A simple method for selection of all such secondary variables $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \ldots$ induced by the root variable $\boldsymbol{\xi}$ and corresponding to the irreps $\Gamma_{\eta_1}, \Gamma_{\eta_2}, \ldots$, follows immediately from the Theorem. It is convenient to rename the secondary variables $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \ldots$ associated with the primary variable $\boldsymbol{\xi}$ as follows: $\boldsymbol{\xi}', \boldsymbol{\xi}'', \ldots$. The complete set of dynamical variables $B_\xi = \{\boldsymbol{\xi}(\text{root}), \boldsymbol{\xi}', \boldsymbol{\xi}'', \boldsymbol{\xi}''', \ldots(\text{secondary})\}$ excited in the physical system will be called a **bush** generated by the root variable $\boldsymbol{\xi}$. A bush of dynamical variables (or bush of modes) determines a certain type of free vibration of the nonlinear system.

Each variable can be considered a root variable which generates its own bush. Let

B_ξ and B_ζ be such bushes whose root variables do not belong to each other, i.e., $\boldsymbol{\xi} \notin B_\zeta$ and $\boldsymbol{\zeta} \notin B_\xi$. Nevertheless, these two bushes are overlapping — they always contain a number of common variables. (At least the variable corresponding to the identity irrep is a part of both bushes.) If $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ are excited simultaneously the vibration of the system is characterized by a new indivisible bush $B_{\xi\zeta}$, which differs from the simple union of B_ξ and B_ζ. Indeed, the bush $B_{\xi\zeta}$ may contain variables belonging to neither B_ξ nor B_ζ.

4 Classification of bushes of normal modes

The group-theoretical method for finding bushes of normal modes for crystals characterized by any space group was developed in [1]. A detailed description of the method used in the program ISOTROPY [12] was given in [13]. We applied the above method for many complex mechanical structures and found that it is useful to classify bushes of vibrational modes using the idea of "classes of dynamical universality". Indeed, the dynamics of a given bush is described by a certain Hamiltonian expressed in terms of modes contained in it, and these dynamics correspond to that of a Hamiltonian system of a generally much lesser dimensionality as compared to the original mechanical system. It is essential to note that Hamiltonians of one and the same type often correspond to very different vibrational bushes and, therefore, they can be classified by certain classes which we call classes of bush universality. The effectiveness of such classification can be illustrated by the example of the class denoted in [13] as B1 (and as B4 in [2]), which comprises two-dimensional bushes of mechanical systems for practically all point and space groups. Moreover, many different nonlinear vibrations can correspond to this class of universality even for the same symmetry group. For example, about 100 different vibrational bushes were found by us in the class B1 for crystals with space group $G_0 = I4/mmm$.

If the Hamiltonian of a given bush is considered to be an analytical function of its arguments up to nonlinear terms of a fixed order, then some of the "exact" classes of universality can be combined into one and the same "approximate" class. Moreover, we can speak of approximate classes of universality B_n of order n, where n is the order of the last nonlinear term of the exact Hamiltonian which is taken into account.

For example, the Hamiltonian for the above mentioned two-dimensional bush B1 up to the terms of the fourth order can be written as follows:

$$H[B1] = (\tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2)+(\tfrac{1}{2}\omega_1^2x_1^2+\tfrac{1}{2}\omega_2^2x_2^2)+(\tfrac{1}{3}Nx_1^3+Kx_1x_2^2)+(\tfrac{1}{4}Ax_1^4+\tfrac{1}{2}Bx_1^2x_2^2+\tfrac{1}{4}Cx_2^4). \quad (7)$$

A complete investigation of bush dynamics even for a bush of small dimensionality can be a very complicated mathematical problem. For example, the above-mentioned class B1 of the two-dimensional bushes, when only terms of up to the third order are taken into account, leads to the so-called generalized Henon-Heiles model which exhibits a complex dynamical behavior, in particular, the chaotic one [21]. (The ordinary Henon-Heiles Hamiltonian can be obtained from that of the bush class B1 by setting $\omega_1 = \omega_2$, $K = -N$ and $A = B = C = 0$ in (7)). The search for the "basic" models of a small dimensionality which will require a thorough mathematical investigation is, in our view, a topical problem of nonlinear dynamics. Therefore, we consider that the singling out of all possible classes of universality for bushes of small dimensionality for all mechanical systems with any of the 230 space symmetry groups is an important task.

The first step in this direction is presented below: we list all bushes of vibrational modes whose dimensionality do not exceed three for all mechanical systems with any of the 32 point groups of crystallographic symmetry. In particular, we consider free molecules as concrete examples of these systems. After a thorough search, we find 9 one-dimensional bushes that all belong to the same class, 73 two-dimensional bushes that belong to 3 distinct classes, and 281 three-dimensional bushes that belong to 7 distinct classes. All of these bushes along with the classes to which they belong are listed in Table 1. (This list was first published in [22]. Differences between the results here and in [22] are due to errors in [22].) Let us explain the crystallographic notation used in the table.

In column 1, we give the point group (PG) of the molecule using the international symbols [23].

In column 2, we give the positions of the atoms in the molecule. We use the notation for Wyckoff positions of atoms in crystals. These Wyckoff positions are listed in [23] for each of the 230 crystallographic space groups. For point group 1, we use the Wyckoff positions for space group $P1$. For point group $\bar{1}$, we use space group $P\bar{1}$, etc. As can be seen in these examples, the space group we use in each case can be obtained by adding the symbol P to the front of the symbol for the point group. The only exceptions to this rule are the following: We use the Wyckoff positions in space groups $P312$, $P31m$, $P\bar{3}1mm$, $P\bar{6}m2$ for point groups 32, $3m$, $\bar{3}m$, $\bar{6}2m$, respectively.

As an example, the 12th entry in the table is for a molecule with point group symmetry mmm and with atoms at positions $im(a)$. We look in [23] for the Wyckoff positions in space group #47 $Pmmm$. In Wyckoff position i, the atoms are at $(x, 0, 0)$ and $(-x, 0, 0)$, where x is an arbitrary distance from the center of the molecule. In Wyckoff position m, the atoms are at $(0, y, 0)$ and $(0, -y, 0)$, where y is also an arbitrary distance from the center of the molecule but not equal to x. In Wyckoff position a, an atom is at the center (0,0,0) of the molecule. The symbol a is in parentheses to indicate that the atom at that position does not participate in the modes of the bush and may or may not be present in the molecule. Thus, the molecule in this example is planar with a rhombic shape, an atom at each corner of the rhombus and an optional atom at the center. Atoms in different Wyckoff positions may or may not be the same kind of atom. However, atoms that belong to a single Wyckoff position must be the same kind of atom.

In column 3, we give the point group symmetry (Sym) of the vibrational modes in the bush. The point group in this column is a subgroup of the point group in column 1, since the atomic displacements in the modes may reduce the equilibrium symmetry of the molecule.

In column 4, we give the class to which the bush belongs. The notation is ours. The letters A,B,C refer to one, two, and three-dimensional bushes, respectively. Note that this notation is not the same as that used in [13]. In other words, class B1 in [13] is not the same as class B1 in this paper.

In column 5, we give the dimension of the bush.

In column 6, we give the irreps to which the root modes and secondary modes belong. The root modes are separated from secondary modes by semicolons. If there is no semicolon, then all of the modes are root modes. The notation for point-group irreps is standard (see, for example, [24]). The letters A, B refer to one-dimensional irreps, the letter E refers to two-dimensional irreps, and the letter T refers to three-dimensional irreps. In most cases, all n dimensions of the irrep contribute to the bush. The exceptions are indicated by an n-dimensional vector in parentheses. For example, we find a notation such as $T_{2g}(a, a, a)$. The vector (a, a, a) gives a "direction" along a one-dimensional line in the three-dimensional representation space. The vibration of this mode is represented by oscillations along this line and contributes a single dimension to the bush.

Table 1. One, two, and three-dimensional bushes in free molecules with crystallographic point group symmetry. For each bush, we give the point group symmetry (PG) of the molecule, the positions (Pos) of the atoms, the point-group symmetry (Sym) of the bush, the universality class to which the bush belongs, the dimension (Dim) of the bush, and the irreps to which the root and secondary (Sec) modes belong. These symbols are explained in more detail in the text.

PG	Pos	Sym	Class	Dim	Root;Sec
$4/mmm$	$j(a)$	$4/mmm$	A0	1	A_{1g}
$4/mmm$	$l(a)$	$4/mmm$	A0	1	A_{1g}
$\bar{6}2m$	$j(a)$	$\bar{6}2m$	A0	1	A_1'
$6/mmm$	$j(a)$	$6/mmm$	A0	1	A_{1g}
$6/mmm$	$l(a)$	$6/mmm$	A0	1	A_{1g}
$\bar{4}3m$	$e(a)$	$\bar{4}3m$	A0	1	A_1
$m\bar{3}m$	$e(a)$	$m\bar{3}m$	A0	1	A_{1g}
$m\bar{3}m$	$g(a)$	$m\bar{3}m$	A0	1	A_{1g}
$m\bar{3}m$	$i(a)$	$m\bar{3}m$	A0	1	A_{1g}
$mm2$	ae	$mm2$	B0	2	A_1, A_1
$mm2$	ag	$mm2$	B0	2	A_1, A_1
mmm	$im(a)$	mmm	B0	2	A_g, A_g
mmm	$iq(a)$	mmm	B0	2	A_g, A_g
mmm	$mq(a)$	mmm	B0	2	A_g, A_g
mmm	$u(a)$	mmm	B0	2	A_g, A_g
mmm	$w(a)$	mmm	B0	2	A_g, A_g
mmm	$y(a)$	mmm	B0	2	A_g, A_g
$4mm$	ad	$4mm$	B0	2	A_1, A_1
$4mm$	ae	$4mm$	B0	2	A_1, A_1
$\bar{4}2m$	$n(a)$	$\bar{4}2m$	B0	2	A_1, A_1
$4/mmm$	$j(a)$	mmm	B1	2	$B_{1g}; A_{1g}$
$4/mmm$	$l(a)$	mmm	B1	2	$B_{1g}; A_{1g}$
$4/mmm$	$j(a)$	mmm	B1	2	$B_{2g}; A_{1g}$
$4/mmm$	$l(a)$	mmm	B1	2	$B_{2g}; A_{1g}$
$4/mmm$	aj	$4mm$	B1	2	$A_{2u}; A_{1g}$
$4/mmm$	al	$4mm$	B1	2	$A_{2u}; A_{1g}$
$4/mmm$	$j(a)$	$\bar{4}2m$	B1	2	$B_{1u}; A_{1g}$
$4/mmm$	$l(a)$	$\bar{4}2m$	B1	2	$B_{2u}; A_{1g}$
$4/mmm$	$gj(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$jj(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$gl(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$jl(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$ll(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$p(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$r(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$4/mmm$	$s(a)$	$4/mmm$	B0	2	A_{1g}, A_{1g}
$3m$	ac	$3m$	B0	2	A_1, A_1
$\bar{3}m$	$k(a)$	$\bar{3}m$	B0	2	A_{1g}, A_{1g}

PG	Pos	Sym	Class	Dim	Root;Sec
$6mm$	ad	$6mm$	B0	2	A_1, A_1
$6mm$	ae	$6mm$	B0	2	A_1, A_1
$\bar{6}2m$	j	$mm2$	B2	2	$E'(a,0); A'_1$
$\bar{6}2m$	aj	$3m$	B1	2	$A''_2; A'_1$
$\bar{6}2m$	$gj(a)$	$\bar{6}2m$	B0	2	A'_1, A'_1
$\bar{6}2m$	$jj(a)$	$\bar{6}2m$	B0	2	A'_1, A'_1
$\bar{6}2m$	$l(a)$	$\bar{6}2m$	B0	2	A'_1, A'_1
$\bar{6}2m$	$n(a)$	$\bar{6}2m$	B0	2	A'_1, A'_1
$6/mmm$	$j(a)$	$\bar{3}m$	B1	2	$B_{1g}; A_{1g}$
$6/mmm$	$l(a)$	$\bar{3}m$	B1	2	$B_{2g}; A_{1g}$
$6/mmm$	aj	$6mm$	B1	2	$A_{2u}; A_{1g}$
$6/mmm$	al	$6mm$	B1	2	$A_{2u}; A_{1g}$
$6/mmm$	$j(a)$	$\bar{6}2m$	B1	2	$B_{1u}; A_{1g}$
$6/mmm$	$l(a)$	$\bar{6}2m$	B1	2	$B_{1u}; A_{1g}$
$6/mmm$	$j(a)$	$\bar{6}2m$	B1	2	$B_{2u}; A_{1g}$
$6/mmm$	$l(a)$	$\bar{6}2m$	B1	2	$B_{2u}; A_{1g}$
$6/mmm$	$ej(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$jj(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$el(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$jl(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$ll(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$n(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$o(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$6/mmm$	$p(a)$	$6/mmm$	B0	2	A_{1g}, A_{1g}
$m\bar{3}$	$j(a)$	$m\bar{3}$	B0	2	A_g, A_g
$\bar{4}3m$	$e(a)$	$\bar{4}2m$	B2	2	$E(a,0); A_1$
$\bar{4}3m$	e	$3m$	B2	2	$T_2(a,a,a); A_1$
$\bar{4}3m$	$ee(a)$	$\bar{4}3m$	B0	2	A_1, A_1
$\bar{4}3m$	$ef(a)$	$\bar{4}3m$	B0	2	A_1, A_1
$\bar{4}3m$	$i(a)$	$\bar{4}3m$	B0	2	A_1, A_1
$m\bar{3}m$	$e(a)$	$4/mmm$	B2	2	$E_g(a,0); A_{1g}$
$m\bar{3}m$	$g(a)$	$4/mmm$	B2	2	$E_g(a,0); A_{1g}$
$m\bar{3}m$	$e(a)$	$\bar{3}m$	B2	2	$T_{2g}(a,a,a); A_{1g}$
$m\bar{3}m$	$i(a)$	$m\bar{3}$	B1	2	$A_{2g}; A_{1g}$
$m\bar{3}m$	$g(a)$	$\bar{4}3m$	B1	2	$A_{2u}; A_{1g}$
$m\bar{3}m$	$i(a)$	$\bar{4}3m$	B1	2	$A_{2u}; A_{1g}$
$m\bar{3}m$	$ee(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$eg(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$gg(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$ei(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$gi(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$ii(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$k(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
$m\bar{3}m$	$m(a)$	$m\bar{3}m$	B0	2	A_{1g}, A_{1g}
m	aaa	m	C0	3	A', A', A'
$2/m$	$mm(a)$	$2/m$	C0	3	A_g, A_g, A_g

PG	Pos	Sym	Class	Dim	Root;Sec
222	$u(a)$	222	C0	3	A, A, A
$mm2$	ae	m	C1	3	$B_1; A_1, A_1$
$mm2$	ag	m	C1	3	$B_2; A_1, A_1$
$mm2$	aae	$mm2$	C0	3	A_1, A_1, A_1
$mm2$	ee	$mm2$	C0	3	A_1, A_1, A_1
$mm2$	aag	$mm2$	C0	3	A_1, A_1, A_1
$mm2$	eg	$mm2$	C0	3	A_1, A_1, A_1
$mm2$	gg	$mm2$	C0	3	A_1, A_1, A_1
$mm2$	ai	$mm2$	C0	3	A_1, A_1, A_1
mmm	$im(a)$	$2/m$	C1	3	$B_{1g}; A_g, A_g$
mmm	$y(a)$	$2/m$	C1	3	$B_{1g}; A_g, A_g$
mmm	$iq(a)$	$2/m$	C1	3	$B_{2g}; A_g, A_g$
mmm	$w(a)$	$2/m$	C1	3	$B_{2g}; A_g, A_g$
mmm	$mq(a)$	$2/m$	C1	3	$B_{3g}; A_g, A_g$
mmm	$u(a)$	$2/m$	C1	3	$B_{3g}; A_g, A_g$
mmm	$u(a)$	222	C1	3	$A_u; A_g, A_g$
mmm	$w(a)$	222	C1	3	$A_u; A_g, A_g$
mmm	$y(a)$	222	C1	3	$A_u; A_g, A_g$
mmm	im	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	iq	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	mq	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	u	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	w	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	ay	$mm2$	C1	3	$B_{1u}; A_g, A_g$
mmm	im	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	iq	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	mq	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	au	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	w	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	y	$mm2$	C1	3	$B_{3u}; A_g, A_g$
mmm	im	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	iq	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	mq	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	u	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	aw	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	y	$mm2$	C1	3	$B_{2u}; A_g, A_g$
mmm	$iim(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$imm(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$iiq(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$imq(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$mmq(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$iqq(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$mqq(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$iu(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$mu(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$qu(a)$	mmm	C0	3	A_g, A_g, A_g

PG	Pos	Sym	Class	Dim	Root;Sec
mmm	$iw(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$mw(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$qw(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$iy(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$my(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$qy(a)$	mmm	C0	3	A_g, A_g, A_g
mmm	$\alpha(a)$	mmm	C0	3	A_g, A_g, A_g
$4/m$	$jj(a)$	$4/m$	C0	3	A_g, A_g, A_g
422	$p(a)$	422	C0	3	A_1, A_1, A_1
$4mm$	ad	$mm2$	C1	3	$B_1; A_1, A_1$
$4mm$	ae	$mm2$	C1	3	$B_2; A_1, A_1$
$4mm$	aad	$4mm$	C0	3	A_1, A_1, A_1
$4mm$	dd	$4mm$	C0	3	A_1, A_1, A_1
$4mm$	aae	$4mm$	C0	3	A_1, A_1, A_1
$4mm$	de	$4mm$	C0	3	A_1, A_1, A_1
$4mm$	ee	$4mm$	C0	3	A_1, A_1, A_1
$4mm$	ag	$4mm$	C0	3	A_1, A_1, A_1
$\bar{4}2m$	$n(a)$	222	C1	3	$B_1; A_1, A_1$
$\bar{4}2m$	n	$mm2$	C1	3	$B_2; A_1, A_1$
$\bar{4}2m$	$gn(a)$	$\bar{4}2m$	C0	3	A_1, A_1, A_1
$\bar{4}2m$	$in(a)$	$\bar{4}2m$	C0	3	A_1, A_1, A_1
$\bar{4}2m$	$o(a)$	$\bar{4}2m$	C0	3	A_1, A_1, A_1
$4/mmm$	$j(a)$	$2/m$	C2	3	$B_{1g}, B_{2g}; A_{1g}$
$4/mmm$	$l(a)$	$2/m$	C2	3	$B_{1g}, B_{2g}; A_{1g}$
$4/mmm$	$j(a)$	222	C2	3	$B_{1g}, B_{1u}; A_{1g}$
$4/mmm$	$l(a)$	222	C2	3	$B_{2g}, B_{2u}; A_{1g}$
$4/mmm$	aj	$mm2$	C2	3	$B_{1g}, A_{2u}; A_{1g}$
$4/mmm$	l	$mm2$	C2	3	$B_{1g}, B_{2u}; A_{1g}$
$4/mmm$	j	$mm2$	C3	3	$E_u(a, 0); A_{1g}, B_{1g}$
$4/mmm$	l	$mm2$	C3	3	$E_u(a, 0); A_{1g}, B_{1g}$
$4/mmm$	j	$mm2$	C2	3	$B_{2g}, B_{1u}; A_{1g}$
$4/mmm$	al	$mm2$	C2	3	$B_{2g}, A_{2u}; A_{1g}$
$4/mmm$	j	$mm2$	C3	3	$E_u(a, a); A_{1g}, B_{2g}$
$4/mmm$	l	$mm2$	C3	3	$E_u(a, a); A_{1g}, B_{2g}$
$4/mmm$	$gj(a)$	mmm	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$4/mmm$	$gl(a)$	mmm	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$4/mmm$	$r(a)$	mmm	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$4/mmm$	$gj(a)$	mmm	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$gl(a)$	mmm	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$s(a)$	mmm	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$jj(a)$	$4/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$jl(a)$	$4/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$ll(a)$	$4/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$p(a)$	$4/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$4/mmm$	$p(a)$	422	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$4/mmm$	$r(a)$	422	C1	3	$A_{1u}; A_{1g}, A_{1g}$

PG	Pos	Sym	Class	Dim	Root;Sec
$4/mmm$	$s(a)$	422	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$4/mmm$	gj	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	jj	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	gl	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	jl	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	ll	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	ap	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	r	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	s	$4mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$4/mmm$	$gj(a)$	$\bar{4}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$4/mmm$	$jl(a)$	$\bar{4}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$4/mmm$	$p(a)$	$\bar{4}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$4/mmm$	$s(a)$	$\bar{4}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$4/mmm$	$gl(a)$	$\bar{4}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$4/mmm$	$jl(a)$	$\bar{4}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$4/mmm$	$p(a)$	$\bar{4}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$4/mmm$	$r(a)$	$\bar{4}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$4/mmm$	$ggj(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gjj(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$jjj(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$ggl(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gjl(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$jjl(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gll(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$jll(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$lll(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gp(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$jp(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$lp(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gr(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$jr(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$lr(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$gs(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$js(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$ls(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$4/mmm$	$u(a)$	$4/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
32	$l(a)$	32	C0	3	A_1, A_1, A_1
$3m$	aac	$3m$	C0	3	A_1, A_1, A_1
$3m$	cc	$3m$	C0	3	A_1, A_1, A_1
$3m$	ad	$3m$	C0	3	A_1, A_1, A_1
$\bar{3}m$	$k(a)$	32	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$\bar{3}m$	k	$3m$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$\bar{3}m$	$ek(a)$	$\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$\bar{3}m$	$ik(a)$	$\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$\bar{3}m$	$l(a)$	$\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$\bar{6}$	$jj(a)$	$\bar{6}$	C0	3	A', A', A'

PG	Pos	Sym	Class	Dim	Root;Sec
$\bar{6}2m$	j	m	C4	3	$E'; A_1'$
$\bar{6}2m$	aj	$mm2$	C5	3	$E'(a,0), E'(a,0); A_1'$
$\bar{6}2m$	$l(a)$	32	C1	3	$A_1''; A_1', A_1'$
$\bar{6}2m$	$n(a)$	32	C1	3	$A_1''; A_1', A_1'$
$\bar{6}2m$	gj	$3m$	C1	3	$A_2''; A_1', A_1'$
$\bar{6}2m$	jj	$3m$	C1	3	$A_2''; A_1', A_1'$
$\bar{6}2m$	al	$3m$	C1	3	$A_2''; A_1', A_1'$
$\bar{6}2m$	n	$3m$	C1	3	$A_2''; A_1', A_1'$
$\bar{6}2m$	$jj(a)$	$\bar{6}$	C1	3	$A_2'; A_1', A_1'$
$\bar{6}2m$	$l(a)$	$\bar{6}$	C1	3	$A_2'; A_1', A_1'$
$\bar{6}2m$	$ggj(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$gjj(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$jjj(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$gl(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$jl(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$gn(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$jn(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$\bar{6}2m$	$o(a)$	$\bar{6}2m$	C0	3	A_1', A_1', A_1'
$6/mmm$	$j(a)$	mmm	C5	3	$E_{2g}(a,0), E_{2g}(a,0); A_{1g}$
$6/mmm$	$l(a)$	mmm	C5	3	$E_{2g}(a,0), E_{2g}(a,0); A_{1g}$
$6/mmm$	$j(a)$	32	C2	3	$B_{1g}, B_{1u}; A_{1g}$
$6/mmm$	$l(a)$	32	C2	3	$B_{2g}, B_{2u}; A_{1g}$
$6/mmm$	j	$3m$	C2	3	$B_{1g}, B_{2u}; A_{1g}$
$6/mmm$	al	$3m$	C2	3	$A_{2u}, B_{2u}; A_{1g}$
$6/mmm$	aj	$3m$	C2	3	$A_{2u}, B_{1u}; A_{1g}$
$6/mmm$	l	$3m$	C2	3	$B_{2g}, B_{1u}; A_{1g}$
$6/mmm$	$ej(a)$	$\bar{3}m$	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$6/mmm$	$jl(a)$	$\bar{3}m$	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$6/mmm$	$o(a)$	$\bar{3}m$	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$6/mmm$	$p(a)$	$\bar{3}m$	C1	3	$B_{1g}; A_{1g}, A_{1g}$
$6/mmm$	$el(a)$	$\bar{3}m$	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$jl(a)$	$\bar{3}m$	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$n(a)$	$\bar{3}m$	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$p(a)$	$\bar{3}m$	C1	3	$B_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$j(a)$	$\bar{6}$	C2	3	$B_{1u}, B_{2u}; A_{1g}$
$6/mmm$	$l(a)$	$\bar{6}$	C2	3	$B_{1u}, B_{2u}; A_{1g}$
$6/mmm$	$jj(a)$	$6/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$jl(a)$	$6/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$ll(a)$	$6/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$p(a)$	$6/m$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$6/mmm$	$n(a)$	622	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$6/mmm$	$o(a)$	622	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$6/mmm$	$p(a)$	622	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$6/mmm$	ej	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	jj	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	el	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$

PG	Pos	Sym	Class	Dim	Root;Sec
$6/mmm$	jl	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	ll	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	n	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	o	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	ap	$6mm$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$6/mmm$	$ej(a)$	$\bar{6}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$6/mmm$	$el(a)$	$\bar{6}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$6/mmm$	$n(a)$	$\bar{6}2m$	C1	3	$B_{1u}; A_{1g}, A_{1g}$
$6/mmm$	$ej(a)$	$\bar{6}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$6/mmm$	$el(a)$	$\bar{6}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$6/mmm$	$o(a)$	$\bar{6}2m$	C1	3	$B_{2u}; A_{1g}, A_{1g}$
$6/mmm$	$eej(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$ejj(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jjj(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$eel(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$ejl(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jjl(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$ell(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jll(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$lll(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$en(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jn(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$ln(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$eo(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jo(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$lo(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$ep(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$jp(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$lp(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
$6/mmm$	$r(a)$	$6/mmm$	C0	3	A_{1g}, A_{1g}, A_{1g}
23	$j(a)$	23	C0	3	A, A, A
$m\bar{3}$	$j(a)$	23	C1	3	$A_u; A_g, A_g$
$m\bar{3}$	$ej(a)$	$m\bar{3}$	C0	3	A_g, A_g, A_g
$m\bar{3}$	$ij(a)$	$m\bar{3}$	C0	3	A_g, A_g, A_g
$m\bar{3}$	$l(a)$	$m\bar{3}$	C0	3	A_g, A_g, A_g
432	$k(a)$	432	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$e(a)$	222	C4	3	$E; A_1$
$\bar{4}3m$	e	$mm2$	C6	3	$T_2(a, 0, 0); A_1, E(-\frac{1}{2}a, -\frac{1}{2}\sqrt{3}a)$
$\bar{4}3m$	ae	$3m$	C5	3	$T_2(a, a, a), T_2(a, a, a); A_1$
$\bar{4}3m$	$i(a)$	23	C1	3	$A_2; A_1, A_1$
$\bar{4}3m$	$eee(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$eef(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$eff(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$ei(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$fi(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1
$\bar{4}3m$	$j(a)$	$\bar{4}3m$	C0	3	A_1, A_1, A_1

PG	Pos	Sym	Class	Dim	Root;Sec
$m\bar{3}m$	$e(a)$	mmm	C4	3	$E_g; A_{1g}$
$m\bar{3}m$	$g(a)$	mmm	C4	3	$E_g; A_{1g}$
$m\bar{3}m$	$e(a)$	mmm	C6	3	$T_{2g}(a,0,0); A_{1g}, E_g(a,0)$
$m\bar{3}m$	$g(a)$	422	C6	3	$E_u(0,a); A_{1g}, E_g(a,0)$
$m\bar{3}m$	e	$4mm$	C6	3	$T_{1u}(a,0,0); A_{1g}, E_g(-\frac{1}{2}a, -\frac{1}{2}\sqrt{3}a)$
$m\bar{3}m$	g	$4mm$	C6	3	$T_{1u}(a,0,0); A_{1g}, E_g(-\frac{1}{2}a, -\frac{1}{2}\sqrt{3}a)$
$m\bar{3}m$	$e(a)$	$\bar{4}2m$	C6	3	$T_{2u}(a,0,0); A_{1g}, E_g(a,0)$
$m\bar{3}m$	$g(a)$	$\bar{4}2m$	C6	3	$T_{2u}(a,0,0); A_{1g}, E_g(a,0)$
$m\bar{3}m$	$i(a)$	$4/mmm$	C5	3	$E_g(a,0), E_g(a,0); A_{1g}$
$m\bar{3}m$	$e(a)$	32	C6	3	$T_{2u}(a,a,a); A_{1g}, T_{2g}(a,a,a)$
$m\bar{3}m$	e	$3m$	C6	3	$T_{1u}(a,a,a); A_{1g}, T_{2g}(a,a,a)$
$m\bar{3}m$	$g(a)$	$\bar{3}m$	C5	3	$T_{2g}(a,a,a), T_{2g}(a,a,a); A_{1g}$
$m\bar{3}m$	$i(a)$	$\bar{3}m$	C5	3	$T_{2g}(a,a,a), T_{2g}(a,a,a); A_{1g}$
$m\bar{3}m$	$i(a)$	23	C2	3	$A_{2g}, A_{2u}; A_{1g}$
$m\bar{3}m$	$ei(a)$	$m\bar{3}$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$m\bar{3}m$	$gi(a)$	$m\bar{3}$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$m\bar{3}m$	$m(a)$	$m\bar{3}$	C1	3	$A_{2g}; A_{1g}, A_{1g}$
$m\bar{3}m$	$k(a)$	432	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$m\bar{3}m$	$m(a)$	432	C1	3	$A_{1u}; A_{1g}, A_{1g}$
$m\bar{3}m$	$eg(a)$	$\bar{4}3m$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$m\bar{3}m$	$ei(a)$	$\bar{4}3m$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$m\bar{3}m$	$k(a)$	$\bar{4}3m$	C1	3	$A_{2u}; A_{1g}, A_{1g}$
$m\bar{3}m$	$eee(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$eeg(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$egg(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$ggg(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$eei(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$egi(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$ggi(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$eii(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$gii(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$iii(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$ek(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$gk(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$ik(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$em(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$gm(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$im(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}
$m\bar{3}m$	$n(a)$	$m\bar{3}m$	C0	3	A_{1g}, A_{1g}, A_{1g}

The actual displacements of the atoms in the vibrational modes are obtained by group-theoretical projection methods, using the irreps listed in column 6. In the example discussed above (12th entry in table), the irrep A_g projects out two independent modes. (That is why A_g is listed twice in column 6.) One of these modes is a "breathing mode" where the atoms oscillate in phase along lines through the center of the molecule. The other mode is similar except that the two atoms in position i are 180° out of phase with the atoms in position m. Neither of these two modes break the mmm symmetry of the molecule. That is why the symmetry of the mode given in column 3 is also mmm.

The Hamiltonian for each bush belonging to the same class has the same form. In particular, the potential energy is written as a sum over polynomials, each invariant with respect to the operations contained in the point group of the molecule. The form of these invariant polynomials are the same for every bush in the class. In the example for class B1 above, the invariant polynomials in (7) are actually all monomials. All bushes belonging to class B1 have Hamiltonians of this form. Only the values of the coefficients $\omega_1, \omega_2, N, K, A, B, C$ depend on the particular bush being considered. We give below the form of the potential energy for each class:

A0: $U = C_1x_1^2 + C_2x_1^3 + C_3x_1^4$

B0: $U = C_1x_1^2 + C_2x_1x_2 + C_3x_2^2 + C_4x_1^3 + C_5x_1^2x_2 + C_6x_1x_2^2 + C_7x_2^3 + C_8x_1^4 + C_9x_1^3x_2 + C_{10}x_1^2x_2^2 + C_{11}x_1x_2^3 + C_{12}x_2^4$

B1: $U = C_1x_1^2 + C_2x_2^2 + C_3x_1^2x_2 + C_4x_2^3 + C_5x_1^4 + C_6x_1^2x_2^2 + C_7x_2^4$

B2: $U = C_1x_2^2 + C_2x_1^2 + C_3x_2^3 + C_4x_1^2x_2 + C_5x_1^3 + C_6x_2^4 + C_7x_1^2x_2^2 + C_8x_1^4 + C_9x_1^3x_2$

C0: $U = C_1x_1^2 + C_2x_1x_2 + C_3x_1x_3 + C_4x_2^2 + C_5x_2x_3 + C_6x_3^2 + C_7x_1^3 + C_8x_1^2x_2 + C_9x_1^2x_3 + C_{10}x_1x_2^2 + C_{11}x_1x_2x_3 + C_{12}x_1x_3^2 + C_{13}x_2^3 + C_{14}x_2^2x_3 + C_{15}x_2x_3^2 + C_{16}x_3^3 + C_{17}x_1^4 + C_{18}x_1^3x_2 + C_{19}x_1^3x_3 + C_{20}x_1^2x_2^2 + C_{21}x_1^2x_2x_3 + C_{22}x_1^2x_3^2 + C_{23}x_1x_2^3 + C_{24}x_1x_2^2x_3 + C_{25}x_1x_2x_3^2 + C_{26}x_1x_3^3 + C_{27}x_2^4 + C_{28}x_2^3x_3 + C_{29}x_2^2x_3^2 + C_{30}x_2x_3^3 + C_{31}x_3^4$

C1: $U = C_1x_1^2 + C_2x_2^2 + C_3x_2x_3 + C_4x_3^2 + C_5x_1^2x_2 + C_6x_1^2x_3 + C_7x_2^3 + C_8x_2^2x_3 + C_9x_2x_3^2 + C_{10}x_3^3 + C_{11}x_1^4 + C_{12}x_1^2x_2^2 + C_{13}x_1^2x_2x_3 + C_{14}x_1^2x_3^2 + C_{15}x_2^4 + C_{16}x_2^3x_3 + C_{17}x_2^2x_3^2 + C_{18}x_2x_3^3 + C_{19}x_3^4$

C2: $U = C_1x_1^2 + C_2x_2^2 + C_3x_3^2 + C_4x_1^2x_3 + C_5x_2^2x_3 + C_6x_3^3 + C_7x_1^4 + C_8x_1^2x_2^2 + C_9x_1^2x_3^2 + C_{10}x_2^4 + C_{11}x_2^2x_3^2 + C_{12}x_3^4$

C3: $U = C_1x_2^2 + C_2x_1^2 + C_3x_3^2 + C_4x_2^3 + C_5x_1^2x_2 + C_6x_2x_3^2 + C_7x_1^2x_3 + C_8x_2^4 + C_9x_1^2x_2^2 + C_{10}x_1^4 + C_{11}x_2^2x_3^2 + C_{12}x_1^2x_3^2 + C_{13}x_3^4 + C_{14}x_1^2x_2x_3$

C4: $U = C_1(x_1^2 + x_2^2) + C_2x_3^2 + C_3(x_1^3 - 3x_1x_2^2) + C_4(x_1^2x_3 + x_2^2x_3) + C_5x_3^3 + C_6(x_1^4 + 2x_1^2x_2^2 + x_2^4) + C_7(x_1^3x_3 - 3x_1x_2^2x_3) + C_8(x_1^2x_3^2 + x_2^2x_3^2) + C_9x_3^4$

C5: $U = C_1x_3^2 + C_2x_1^2 + C_3x_1x_2 + C_4x_2^2 + C_5x_3^3 + C_6x_1^2x_3 + C_7x_1x_2x_3 + C_8x_2^2x_3 + C_9x_1^3 + C_{10}x_1^2x_2 + C_{11}x_1x_2^2 + C_{12}x_2^3 + C_{13}x_3^4 + C_{14}x_1^2x_3^2 + C_{15}x_1^4 + C_{16}x_1x_2x_3^2 + C_{17}x_1^3x_2 + C_{18}x_1^2x_2^2 + C_{19}x_2^2x_3^2 + C_{20}x_1x_2^3 + C_{21}x_2^4 + C_{22}x_1^3x_3 + C_{23}x_1^2x_2x_3 + C_{24}x_1x_2^2x_3 + C_{25}x_2^3x_3$

C6: $U = C_1x_2^2 + C_2x_1^2 + C_3x_3^2 + C_4x_2^3 + C_5x_1^2x_2 + C_6x_2x_3^2 + C_7x_1^2x_3 + C_8x_3^3 + C_9x_2^4 + C_{10}x_1^2x_2^2 + C_{11}x_1^4 + C_{12}x_2^2x_3^2 + C_{13}x_1^2x_3^2 + C_{14}x_3^4 + C_{15}x_1^2x_2x_3 + C_{16}x_2x_3^3$

5 Conclusion

The concept of bushes of modes in non-linear dynamic systems has only recently been introduced and developed. In this paper, we have reviewed the main issues involved. To illustrate this concept, we have presented a complete list of one, two, and three-dimensional bushes for free molecules with crystallographic point-group symmetry. Our analysis also applies to any macroscopic mechanical system with point symmetry as well. We have classified these bushes according to the form of their Hamiltonian. The dynamics of these 363 bushes fall into 11 classes. Bushes in the same class exhibit similar non-linear dynamical behavior. This classification greatly simplifies the problem of understanding the possible non-linear dynamical behavior in a large number of systems.

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