This Week's Citation Classic®

Lea K R, Leask M J M & Wolf W P. The raising of angular momentum degeneracy of *f*-electron terms by cubic crystal fields. *J. Phys. Chem. Solids* 23:1381-405, 1962.
[Clarendon Laboratory, University of Oxford, England]

In those days the Clarendon Laboratory was a world center for research in the magnetic properties of transition metal compounds. Several research groups were looking at microwave absorption spectra of the transition metal ions, both iron group and rare earths. While the ground state properties of such ions could be understood very well in terms of an effective "spin" Hamiltonian approach, a fuller understanding needed information about the optically excited states as well. This meant there was a need to understand the effect on the crystalline environment on the angular momentum states of the ion. Whereas a free ion having angular momentum *J* has isotropic properties, in a crystal the $(2J+1)$-fold degeneracy is removed and this leads to properties that depend very much on direction relative to the crystal axes. [The *SCI*® indicates that this paper has been cited in over 975 publications.]

Crystal Field Effects of Rare Earths

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Professor J.H. Van Vleck, the doyen of all those who have worked in magnetism, happened to be the Eastman Visiting Professor at the University of Oxford in the very early 1960s. Amongst many subjects discussed over cups of coffee in the Clarendon Laboratory, we certainly talked over the possibility of working out once and for all time the effect of a cubic crystal environment on all possible states of rare earth ions. I was a postdoctoral student at the time, my thesis supervisor having been W.P. Wolf. We conceived of this as a joint project, though I clearly recall lukewarm enthusiasm on the part of Wolf! And for good reason; the operation would clearly need a computer, and computers were in their infancy. The final result would be a set of dry-as-dust tables that no one would ever look at or comment upon, unless of course they happened to find an error.

With the Ferranti Mercury computer the university possessed then, a major problem for us was getting to grips with the procedure for diagonalising matrices. Today this is trivial; then it most certainly was not. Fortunately for us, there was just one man in the Clarendon Laboratory who understood how to carry out this most arcane of operations—K.R. Lea. Ken was in the atomic physics group doing quite different research, but gladly agreed to mastermind the computer side of things.

The citation rate for the resulting paper was high straightaway, for the reason that people everywhere started to get interested in the properties of rare earth ions in calcium fluoride, a cubic crystal.[1] The tables and figures in the paper seemed very well suited to the needs of those interested. But there was another factor that I sensed then and have continued to sense for many years. It seemed that for many physicists and chemists, struggling with the very concept of the quantum mechanics of the crystal field, this paper provided the conceptual breakthrough. More than a few people have said to me, when meeting me for the first time, "...Your paper taught me all I needed to know about crystal field effects in rare earths!"

One other factor that mattered was that no one ever reported any errors in the tables. Nowadays, of course, it is utterly straightforward to repeat the calculations for the specific problem in hand, but for over a decade the calculated results in the paper provided the primary source of information for many people. It was just too difficult to program computers to repeat the whole calculation! My strongest recollection of those times is the continuing nightmare of checking the final manuscript, looking for typographical errors.

Finally, one interesting consequence of the diagrams in the paper is the evident occurrence, in particular cases, of quantum-mechanical degeneracy over and above that expected on symmetry grounds alone. This in turn spawned some theoretical activity by us and others,[2,3] since, in general, the occurrence of additional degeneracy usually implies additional symmetry—in this case, quite unexpected.

1. **Sabisky E S.** Paramagnetic resonance of divalent holmium in cubic hosts: CaF_2, SrF_2, BaF_2, and $SrCl_2$. *Phys. Rev.* 141:352-62, 1966. (Cited 30 times.)
2. **Battison J E, Kasten A, Leask M J M & Lowry J B.** High field Zeeman effects in holmium vanadate. *Phys. Lett. A* 55:173-4, 1975. (Cited 10 times.)
3. **Bleaney B, Gregg J F, Hansen P, Huan C H A, Lazzouni M, Leask M J M, Morris I D & Wells M R.** Further studies of the enhanced nuclear magnet $HoVO_4$. I. The crystal field and the Zeeman spectrum. *Proc. Roy. Soc. London Ser. A* 416:63-73, 1988.

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