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镧系元素**f-f**跃迁光谱计算

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摘要 运用不可约张量算符方法,建立了f-f超灵敏跃迁光谱的计算模型,编制了计算f离子^2s+1L~J能级、约化矩阵元、晶体场Stark能级、晶体场态-态跃迁振子强度及模拟吸收光谱的计算机程序.其中,自由f离子能级计算采用包括双电子与叁电子组态相互作用的二三参数模型,晶体场Stark分裂计算采用单电子轨道近似,用Newman角叠加模型计算晶体场参数.f-f跃迁振子强度计算包括静电诱导偶极跃、配体极化偶极跃、振动诱导电偶极跃迁及磁偶极跃迁的贡献.

关键词 计算机应用 计算机模拟 镧系元素 光谱分析 跃迁 不可约表示

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Calculation of the f-f transition spectra of the lanthanides

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Abstract A computational model and corresponding computer program for calculating the 2S+1LJ energy levels, reduced matrix elements, Stark energy levels of crystal field, state-state transition oscillator strength between crystal energy levels, and for modulating the absorption spectrum of f-element were developed based on irreducible tensor operator method. The energy levels of free metallic ion were calculated with a 13 parameters model including the 2-body and 3-body interactions. The Stark energy levels of crystal field were calculated using the model proposed by Newman based on 1 electron orbital approximation The f-f oscillator strength calculation includes the contribution of electrostatic-induced, ligand polarization, vibronic-induced, magnetic dipolar transitions.

Key words COMPUTER APPLICATIONS COMPUTERIZED SIMULATION LANTHANON SPECTROGRAPHIC ANALYSIS TRANSITION IRREDUABLE REPRESENTATION

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