

Library Indian Institute of Science Education and Research Mohali



DSpace@IISERMohali (/jspui/)

- / Thesis & Dissertation (/jspui/handle/123456789/1)
- / Master of Science (/jspui/handle/123456789/2)
- / MS-13 (/jspui/handle/123456789/914)

Please use	this identifier to cite or link to this item: http://hdl.handle.net/123456789/946
Title:	Critical Points and Catastrophes of Molecular Electrostatic potential
Authors:	Ashima (/jspui/browse?type=author&value=Ashima)
Keywords:	Molecular Electrostatic potential Catastrophe Theory Zero Flux Surfaces
Issue Date:	24-Aug-2018
Publisher:	IISERM
Abstract:	The present work deals with the construction of an approach to find critical points of a 3-D scalar field(Molecular Electrotatic Potential). This approach gives an insight to the zero flux surfaces which help us visualize critical points using Euler Characterstic. Along with the marching cubes, some catastrophe theory on some reaction pathways of molecules has also been performed as the transition state has been compared to reactant or product.
URI:	http://hdl.handle.net/123456789/946 (http://hdl.handle.net/123456789/946)
Appears in Collections:	MS-13 (/jspui/handle/123456789/914)

Files in This Item:				
File	Description	Size	Format	
MS13062.pdf (/jspui/bitstream/123456789/946/4/MS13062.pdf)		850.06 kB	Adobe PDF	View/Open (/jspui/bitstream/123456789/946/4/

Show full item record (/jspui/handle/123456789/946?mode=full)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.