

Title (en)
SYSTEM AND METHOD OF COMPUTING AND RENDERING THE NATURE OF POLYATOMIC MOLECULES AND POLYATOMIC MOLECULAR IONS

Title (de)
SYSTEM UND VERFAHREN ZUR BERECHNUNG UND DARSTELLUNG DER NATUR VON POLYATOMAREN MOLEKÜLEN UND IONEN MIT POLYATOMAREN MOLEKÜLEN

Title (fr)
SYSTEME ET PROCEDE DE CALCUL ET DE RENDU DE LA NATURE DE MOLECULES POLYATOMIQUES ET D'IONS MOLECULAIRES POLYATOMIQUES

Publication
EP 1941415 A4 20110105 (EN)

Application
EP 06827305 A 20061030

Priority

- US 2006042692 W 20061030
- US 73088205 P 20051028
- US 73215405 P 20051102
- US 73774405 P 20051118
- US 75852806 P 20060113
- US 78051806 P 20060309
- US 78869406 P 20060404
- US 81259006 P 20060612
- US 81525306 P 20060621

Abstract (en)
[origin: WO2007051078A2] A method and system of physically solving the charge, mass, and current density functions of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species using Maxwell's equations and computing and rendering the physical nature of the chemical bond using the solutions. The results can be displayed on visual or graphical media. The display can be static or dynamic such that electron motion and specie's vibrational, rotational, and translational motion can be displayed in an embodiment. The displayed information is useful to anticipate reactivity and physical properties. The insight into the nature of the chemical bond of at least one specie can permit the solution and display of those of other species to provide utility to anticipate their reactivity and physical properties.

IPC 8 full level
G06F 19/00 (2011.01); **G01N 31/00** (2006.01); **G06F 19/16** (2011.01)

CPC (source: EP)
G16C 20/80 (2019.01); **G16C 10/00** (2019.01)

Citation (search report)

- [ID] WO 2005067678 A2 20050728 - BLACKLIGHT POWER INC [US], et al
- See references of WO 2007051078A2

Designated contracting state (EPC)
AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IS IT LI LT LU LV MC NL PL PT RO SE SI SK TR

DOCDB simple family (publication)
WO 2007051078 A2 20070503; WO 2007051078 A3 20090430; EP 1941415 A2 20080709; EP 1941415 A4 20110105;
WO 2007053486 A2 20070510; WO 2007053486 A3 20090507

DOCDB simple family (application)
US 2006042692 W 20061030; EP 06827305 A 20061030; US 2006042140 W 20061030