Summary of the Research Works of Professor Bahoueddine TANGOUR

This document aims to group my publications into thematic areas:

1) Chemical Reactivity

a) Phosphorus Compounds

I began my research activities in 1975 with a DEA on the formation of monocyclic phosphoranes with P–H bonds through the oxidative addition of alcohols and amines to tricoordinated monocyclic phosphorus compounds. I have continued to explore this topic ever since.

The major findings from the experimental part [1–6] can be summarized as follows:

- The addition remains in the form of a dynamic equilibrium.
- The passage through pentacoordinated phosphorus is a necessary step for any ligand redistribution around tricoordinated compounds.
- Two competing mechanisms occur depending on whether the nucleophile is an alcohol or an amine.

  Several theoretical studies [5–10] validated these results, the most fundamental being the mapping of a potential energy surface with 15 degrees of freedom.

My two PhD theses have been devoted to this topic.

b) Ruthenium Complexes

Several ligand exchange or hydrogenation reactions catalyzed by ruthenium have been the subject of many works in my group [11–20]. The most important results were the identification of competing transition states. We even characterized a transition state with 10 active atoms within the transition state's influence zone. The high catalytic activity of ruthenium was linked to its versatility, defined as its ability to change the nature and role of its atomic orbitals in the transition state.

Three PhD theses have addressed this subject.

c) Supernucleophile Attacks

We studied the reactions of supernucleophiles with benzofurans or thiophene derivatives, covering both the experimental [21,22] and theoretical aspects [23–28]. We highlighted the importance of kinetic vs. thermodynamic competition in these parallel reactions. Using the RIRC technique, developed in our laboratory, we were able to identify hidden intermediates that play a crucial role in the orientation and control of these processes.

Two PhD theses have addressed this subject.

d) CO_2 Capture

The most cited article from my work concerns CO_2 capture [29]. We demonstrated the necessity of a second nucleophilic center to enable amine addition to CO_2. We particularly focused on diamines [30] and on the degradation process of supported amines, elucidating the radical mechanism [31] responsible for oxidation.

e) Other Topics

We also investigated other reactions in the framework of collaborations. Examples include reactions involving copper [32], silver, zinc [33], palladium [34], iron [35], molybdenum [36], germanium [37], natural compounds [38–43], cytochromes [44,45], aziridines [46], proton transfer [47], and microwave activation [48].

Two PhD theses dealt with copper, silver, and zinc on one hand, and cytochromes on the other.

2) Spectroscopy

Several studies addressed theoretical spectroscopy:
a) PF_2H [49]
b) ZnX (X = O, S, Se, Te, Po) [50]
c) ZnO [51]
One PhD thesis was largely based on these works.

3) Nanostructured Materials

Following the works presented during the "Workshop on Nanomaterials and Nanotechnology" that I organized in 2008 in collaboration with the NSF (USA), my team transitioned to nanostructured materials.

a) Nanotubes: We mainly conducted confinement studies inside carbon or TiO_2 nanotubes [52], germanium [53], or BN [54,55]. These studies involved small molecules such as H_2 [56,57], F_2 [58], HX (X = F, Cl, Br, I) [59], H_2O, $(TiO_2)_2$ [60], TiO_2 [61], and C_2H_6 [62].
Two PhD theses focused on carbon and TiO_2 nanotubes.
b) Fullerenes: Two studies dealt with fullerene functionalization [63,64].
c) Graphene: We investigated graphene in its sheet form [65].
d) MOFs: Several studies explored the capture of small molecules in various MOFs [66,67].
One PhD thesis was largely based on these works.
e) Dyes: Our group investigated the activity mechanisms of certain organic dyes [68,69].
Two PhD thesis were largely based on these works.

4) Drug Vectorization

a) Nanotubes: Encapsulation of anticancer [70–73] and anti-HIV drugs [74].
One PhD thesis was largely based on these works.
b) Graphene Nest: One anticancer drug was studied during its entry and exit from a graphene nest [75].
c) Nanocones: Grafting or encapsulation of an anticancer drug was investigated in nanocones [76].
One PhD thesis was largely based on these works.
d) Dendrimers: An anticancer drug was studied inside dendrimer cavities [77].
One PhD thesis was largely based on these works.

5) Machine Learning

This is a new axis, necessary for the evolution of our research lines.
a) Ruthenium complexes: submitted to *Materials Today*.
b) QSAR modeling [39].

References

[1] M.T. Boisdon, C. Malavaud, B. Tangour, J. Barrans, PHOSPHORANES MONOCYCLIQUES A LIGAND HYDROGENE I-ETUDE DE L'EQUILIBRE DE FORMATION, Phosphorous and Sulfur and the Related Elements 8 (1980) 305–313.
[2] B. Tangour, M.T. Boisdon, C. Malavaud, J. Barrans, Addition de composes insatures sur les phosphoranes monocycliques a liaison p-h, Tetrahedron 44 (1988) 6087–6093.
[3] B. Tangour, C. Malavalid, M.T. Boisdon, J. Barrans, FORMATION D'ALCOXY ET ALKYLAMINO DIOXA, OXAZA ET DIAZAPHOSPHORANES MONOCYCLIQUES A LIAISON P-H, Phosphorous and Sulfur and the Related Elements 40 (1988) 33–39.

[4] B. Tangour, C. Malavaud, M.T. Boisdon, J. Barrans, LES PHOSPHORANES MONOCYCLIQUES A LIAISON PH DANS LES REACTIONS DE REDISTRIBUTION DE LIGANDS DES COMPOSES DU PHOSPHORE TRICOORDONNE, Phosphorus, Sulfur, and Silicon and the Related Elements 45 (1989) 189–195.
[5] O. Fliss, A. MEJRI, K. Essalah, M.-T. Boisdon, B. TANGOUR, Étude expérimentale et théorique de la cinétique de l'alcoolyse de la liaison P–N extracyclique du 2-diméthylamino-4,4,5,5-tétraméthyl-1,3-dioxaphospholane monocyclique, Comptes Rendus Chimie 19 (2016) 585–593.
[6] A. MEJRI, O. Fliss, K. Essalah, M.A. BOUGHDIRI, F. Picaud, B. TANGOUR et al., New insights into phosphorus biphilicity: Stereochemistry of monocyclic aminophosphoranes formation, Int. J. Quantum Chem. 123 (2023).
[7] O. Fliss, R. Bessrour, B. TANGOUR, Theoretical DFT study of 1,3,2-dioxa-phosphoranes formation by oxidative addition of methanol on monocyclic phospholanes, Journal of Molecular Structure: THEOCHEM 758 (2006) 225–232.
[8] T. Boubaker, M.-T. Boisdon, R. Bessrour, B. TANGOUR, Kinetic Study of Phosphoranes formation by oxidative addition of aliphatic alcohols on monocyclic Phospholanes, Oriental Journal of Chemistry 2004, 2004 509-514. http://www.orientjchem.org/?p=17931".
[9] M.A. BOUGHDIRI, A. MEJRI, B. TANGOUR, Pentavalent phosphorus formation mechanism, Computational and Theoretical Chemistry 1211 (2022) 113678.
[10] A. Méjri, F. Picaud, M. El Khalifi, T. Gharbi, B. TANGOUR, Controlling activation barrier by carbon nanotubes as nano-chemical reactors, Journal of molecular modeling 23 (2017) 229.
[11] Z. Hosni, B. TANGOUR, S. Achour, A DFT Study of the Hexene Hydrogenation Catalysed by the Complex RuH(CO)(Cl)(PCy3): Monophosphine vs Diphosphine Paths.
[12] S. Achour, Z. Hosni, B. TANGOUR, Hexene hydrogenation catalysed by the complex monohydrid complexes: A DFT study of associated vs dissociated pathways, Journal of molecular graphics & modelling 98 (2020) 107583.
[13] S. Achour, Z. Hosni, B. TANGOUR, Olefin Hydrogenation Mechanism Catalyzed by Ruthenium Complexes Containing N-Heterocyclic Carbene Ligands, SSRN Journal (2022).
[14] S. Achour, M. Seydou, F. Maurel, B. TANGOUR, Intramolecular hydrogenation of triethylsilylethylene catalyzed by Ru(II) complex: Agostic bond formation and trizonal transition states with ten acting atoms, Inorganica Chimica Acta 469 (2018) 536–544.
[15] T. Ayed, B. TANGOUR, J.C. Barthelat, Validation of the ONIOM method in a small system RuH2[eta2HSiMe2)2NH]PMe3)2, Oriental Journal of Chemistry 2005, 2005 29–34.
[16] T. Ayed, J.-C. Barthelat, B. TANGOUR, C. Pradère, B. Donnadieu, M. Grellier et al., Structure and Bonding in a Disilazane Ruthenium Complex. Catalytic Selective Deuteration of Disilazane, Organometallics 24 (2005) 3824–3826.
[17] R. Ben Said, K. Hussein, B. TANGOUR, S. Sabo-Etienne, J.-C. Barthelat, A density functional theory study of dinitrogen bonding in ruthenium complexes, Journal of Organometallic Chemistry 673 (2003) 56–66.
[18] R. Ben Said, K. Hussein, B. TANGOUR, S. Sabo-Etienne, J.-C. Barthelat, A DFT study of germane activation in ruthenium complexes. σ-coordination versus oxidative addition, New J. Chem. 27 (2003) 1385–1391.
[19] R. Ben Said, B. TANGOUR, J.-C. Barthelat, Quantum chemical investigations of intramolecular isomerization in RuH2(CO)2(PMe3)2, Journal of Molecular Structure: THEOCHEM 857 (2008) 115–122.
[20] S. Achour, Z. Hosni, B. TANGOUR, Hydrogenation of hexene catalyzed by a ruthenium (II) complex with N -heterocyclic carbene ligands, Int. J. Quantum Chem. 124 (2024).
[21] T. Boubaker, A.P. Chatrousse, F. Terrier, B. TANGOUR, J.M. Dust, E. Buncel, Water and hydroxide ion pathways in the σ-complexation of superelectrophilic 2-aryl-4,6-dinitrobenzotriazole 1-

oxides in aqueous solution. A kinetic and thermodynamic study, J. Chem. Soc., Perkin Trans. 2 (2002) 1627–1633.
[22] W. Gabsi, K. Essalah, R. Goumont, B. TANGOUR, T. Boubaker, The ambident electrophilic behavior of 5-nitro-3-X-thiophenes in σ-complexation processes, Int. J. Chem. Kinet. 50 (2018) 659–669.
[23] M.A. BOUGHDIRI, T. Boubaker, B. TANGOUR, Theoretical investigation of methoxide ion reaction on the 7-methyl-4,6-dinitrobenzofuroxan, Can. J. Chem. 94 (2016) 699–703.
[24] M.A. BOUGHDIRI, O. Fliss, T. Boubaker, B. TANGOUR, Theoretical Thermodynamic Study of the Unexpected Stability and Electrophily of the 7-Methyl 4,6 Dinitro Benzofuroxane (DNBF), Oriental Journal of Chemistry 463-498. http://www.orientjchem.org/?p=19549.
[25] M.A. BOUGHDIRI, O. Fliss, T. Boubaker, B. TANGOUR, Theoretical Study of the Kinetic-Thermodynamic Competition between the σ-Complexes Obtained by the Reaction of the Methoxy Ion on the 7- Methyl 4-Nitro Benzofuroxan, Biosciences Biotechnology Research Asia 2006, 2006 317–322. https://bit.ly/30ISlwI.
[26] M.A. BOUGHDIRI, B. TANGOUR, T. Boubaker, Theoretical and experimental reinvestigation of methoxide ion reaction with 7-methyl 4-nitro benzofuroxan, J. Theor. Comput. Chem. 15 (2016) 1650030.
[27] A. SMAOUI, K. Essalah, X. Assfeld, G. Herlem, F. Picaud, B. TANGOUR, Authorea.
[28] A. SMAOUI, K. Essalah, T. Boubaker, X. Assfeld, F. Picaud, B. Tangour, First-principles study of the reaction mechanism governing the SNAr of the dimethylamine on 2-methoxy-5-nitrothiophenes, Theor Chem Acc 139 (2020).
[29] R.B. Said, J.M. Kolle, K. Essalah, B. TANGOUR, A. Sayari, A Unified Approach to CO2-Amine Reaction Mechanisms, ACS omega 5 (2020) 26125–26133.
[30] R.B. Said, S. Rahali, C. Yan, M. Seydou, B. TANGOUR, A. Sayari, CO2 Capture by Diamines in Dry and Humid Conditions: A Theoretical Approach, The journal of physical chemistry. A 127 (2023) 7756–7763.
[31] I. Abidli, B. TANGOUR, A. Sayari, Mechanistic insights into the oxidative degradation of amine-containing CO2 adsorbents, Environmental research 275 (2025) 121445.
[32] O. Bouhlel, M. Zina, S. Boughdiri, B. Tangour, Theoretical ab initio study of NO and CO depollution reaction catalyzed by copper, Int. J. Quantum Chem. 84 (2001) 623–629.
[33] O. Bouhlel, S. Boughdiri, O. Fliss, B. Tangour, Theoretical ab initio study of NO and CO depollution reaction catalyzed by zinc, Journal of Molecular Structure: THEOCHEM 571 (2001) 191–199.
[34] T. Ayed, N. Guihéry, B. TANGOUR, J.-C. Barthelat, Theoretical Study of the Metal–Metal Interaction in Dipalladium(I) Complexes, Theor Chem Acc 116 (2006) 497–504.
[35] A. Dhouib, K. Essalah, B. Tangour, M. Abderrabba, A DFT study of monophosphate complexes of iron (III) Fe(H2PO4)(H2O)m2+ (m=3, 4, 5), Journal of Molecular Structure: THEOCHEM 715 (2005) 125–131.
[36] A. Dhouib, K. Essalah, B. Tangour, M. Abderraba, Gyroscopic tensor ab initio calculation of the molecular crystals: (Mo6X14)2?Y?(TTF+)3 (X=Br, Cl andY=Br, Cl, I), Int. J. Quantum Chem. 87 (2002) 220–224.
[37] S. Boughdiri, K. Hussein, B. TANGOUR, M. Dahrouch, M. Rivière-Baudet, J.-C. Barthelat, Aromaticity or non aromaticity in germanazenes? Theoretical studies on germanazenes, the N-cyano analogs and their carbodiimide isomers, Journal of Organometallic Chemistry 689 (2004) 3279–3286.
[38] R.B. Said, S. Rahali, M.A.B. Aissa, I.B. Abdel-Farid, A.A. Mohamed, B. TANGOUR et al., Fingerprinting profile of flavonol glycosides from Bassia eriophora using negative electrospray ionization, computational studies and their antioxidant activities, Journal of Molecular Structure 1241 (2021) 130689.

[39] R.B. Said, R. Hanachi, S. Rahali, M.A.M. Alkhalifah, F. Alresheedi, B. TANGOUR et al., Evaluation of a new series of pyrazole derivatives as a potent epidermal growth factor receptor inhibitory activity: QSAR modeling using quantum-chemical descriptors, Journal of computational chemistry 42 (2021) 2306–2320.
[40] I.S. Al Nasr, R. Hanachi, R.B. Said, S. Rahali, B. TANGOUR, S.I. Abdelwahab et al., p-Trifluoromethyl- and p-pentafluorothio-substituted curcuminoids of the 2,6-di(E)-benzylidene)cycloalkanone type: Syntheses and activities against Leishmania major and Toxoplasma gondii parasites, Bioorganic chemistry 114 (2021) 105099.
[41] R. Ben Said, M.A. Ben Aissa, S. Rahali, B. TANGOUR, M. Kowalczyk, W. Oleszek et al., Fingerprinting of two an acylated polyoxypregnane glycosides from Caralluma quadrangula (Forssk.) N.E.Br. using UPLC-ESI-Q-TOF and computational study, Natural product research (2021) 1–5.
[42] R. Ben Said, A.I. Hamed, K. Essalah, A.S. Al-Ayed, S. Boughdiri, B. TANGOUR et al., Fast characterization of C- glycoside acetophenones in Medemia argun male racemes (an Ancient Egyptian palm) using LC-MS analyses and computational study with their antioxidant effect, Journal of Molecular Structure 1145 (2017) 230–239.
[43] R. Hanachi, R. Ben Said, H. Allal, S. Rahali, M.A.M. Alkhalifah, F. Alresheedi et al., Structural, QSAR, machine learning and molecular docking studies of 5-thiophen-2-yl pyrazole derivatives as potent and selective cannabinoid-1 receptor antagonists, New J. Chem. 45 (2021) 17796–17807.
[44] L. Benkaidali, F. André, G. Moroy, B. TANGOUR, F. Maurel, M. Petitjean, The Cytochrome P450 3A4 has three Major Conformations: New Clues to Drug Recognition by this Promiscuous Enzyme, Molecular informatics 36 (2017).
[45] L. Benkaidali, F. André, G. Moroy, B. TANGOUR, F. Maurel, M. Petitjean, Four Major Channels Detected in the Cytochrome P450 3A4: A Step toward Understanding Its Multispecificity, International journal of molecular sciences 20 (2019).
[46] N. Besbes, T. Ayed, P. Pale, B. TANGOUR, Réarrangement thermique de N-acyl-2,2-diméthylaziridines substituées: Une étude mécanistique, Comptes Rendus Chimie 11 (2008) 1283–1288.
[47] H. Abdeldjebar, Y. Belmiloud, W. Djitli, S. Achour, M. Brahimi, B. TANGOUR, Proton transfer in the benzimidazolone and benzimidazolthione tautomerism process catalyzed by polar protic solvents, Progress in Reaction Kinetics and Mechanism 44 (2019) 143–156.
[48] A. Telmoudi, F. M'Henni, B. TANGOUR, Synthesis of acid 2,9-di-(ortho-hydroxyphenoxy) sebacic by microwaves activation technique, Oriental Journal of Chemistry 2005, 2005 213-217. http://www.orientjchem.org/?p=19049.
[49] B. Tangour, M. Ben Caid, J.C. Barthelat, Ab initio study of some spectroscopic properties of PF2H, Journal of Molecular Structure: THEOCHEM 235 (1991) 399–408.
[50] S. Boughdiri, M. Dachraoui, B. TANGOUR, Electronic properties study of ZnX (1S+) molecules (X= O, S, Se Te Po), Oriental Journal of Chemistry 235-240. http://www.orientjchem.org/?p=19059.
[51] S. Boughdiri, B. TANGOUR, C. Teichteil, J.-C. Barthelat, T. Leininger, Revisiting the nature of the ZnO ground state: Influence of spin–orbit coupling, Chemical Physics Letters 462 (2008) 18–22.
[52] S. Dargouthi, C. Minot, B. TANGOUR, Structural study of TiO2 nanotube based to the (101) anatase surface, Superlattices and Microstructures 102 (2017) 307–313.
[53] W. Djitli, M.L. Abdelatif, Y. Belmiloud, H. Abdeldjebar, M. Brahimi, B. TANGOUR, H2 storage by confinement inside germanium nanotubes, Superlattices and Microstructures 122 (2018) 596–607.
[54] Y.F.Z. Assas, Y. Belmiloud, M.L. Abdelatif, S. Abtouche, M. Brahimi, B. Tangour, Fluorine and chlorine gas storage by confinement inside boron nitrogen nanotubes, Indian Journal of chemistry 2021, 2021 1192–1200.

[55] F.Z. Assas, Y. Belmiloud, M.L. Abdelatif, M. Sehailia, A. Rabahi, M. Brahimi et al., New Insights in the Use of Boron Nitrogen Nanotubes as Cisplatin Nanovector, Physical Chemistry Research 2023, 2023 253–265.
[56] Y. Belmiloud, W. Djitli, H. Abdeldjebar, M.L. Abdelatif, B. TANGOUR, M. Brahimi, First principles calculations of a H 2 molecule inside boron-nitrogen nanotubes, Superlattices and Microstructures 101 (2017) 547–558.
[57] W.F. Gtari, B. TANGOUR, A theoretical study of the dihydrogen molecule confined inside carbon nanotubes, Int. J. Quantum Chem. 113 (2013) 2397–2404.
[58] W. Felah Gtari, B. TANGOUR, F 2 storage by confinement inside carbon nanotubes, Can. J. Chem. 94 (2016) 15–19.
[59] W.F. Gtari, B. TANGOUR, Interaction of HF, HBr, HCl and HI Molecules with Carbon Nanotubes, Acta chimica Slovenica 65 (2018) 289–295.
[60] S. Dargouthi, S. Boughdiri, B. TANGOUR, Stabilizing of the Transitory Species (TiO2)2 by Encapsulation Into Carbon Nanotubes, Acta chimica Slovenica 62 (2015) 445–451.
[61] S. Dargouthi, S. Boughdiri, B. TANGOUR, Stability of TiO2 Molecule Confined Inside a Carbon Nanotube: A Theoretical Study, j comput theor nanosci 11 (2014) 1258–1263.
[62] A. Gannouni, M. Ouraghi, S. Boughdiri, R. Bessrour, A. Benaboura, B. TANGOUR, C6H2@ Single Walled Carbon Nanotube First Principle Theoretical Study: Equivalent Temperature Confinement Effect of Carbon Nanotubes, j comput theor nanosci 9 (2012) 379–383.
[63] H. Khemir, B. TANGOUR, F. Moussa, In Silico Study of Spacer Arm Length Influence on Drug Vectorization by Fullerene C 60, Journal of Nanomaterials 2015 (2015) 1–8.
[64] M.B. Messaouda, F. Moussa, B. TANGOUR, H. Szwarc, M. Abderrabba, Addition of bio-organic compounds on C60: A semi-empirical investigation of its reactivity with glycine, Journal of Molecular Structure: THEOCHEM 809 (2007) 153–159.
[65] S. Rahali, Y. Belhocine, J. Touzeau, B. TANGOUR, F. Maurel, M. Seydou, Balance between physical and chemical interactions of second-row diatomic molecules with graphene sheet, Superlattices and Microstructures 102 (2017) 45–55.
[66] S. Rahali, M. Seydou, Y. Belhocine, F. Maurel, B. TANGOUR, First-principles investigation of hydrogen storage on lead(II)-based metal-organic framework, International Journal of Hydrogen Energy 41 (2016) 2711–2719.
[67] S. Rahali, Y. Belhocine, M. Seydou, F. Maurel, B. TANGOUR, Multiscale study of the structure and hydrogen storage capacity of an aluminum metal-organic framework, International Journal of Hydrogen Energy 42 (2017) 15271–15282.
[68] S. Trabelsi, N. Kouki, M. Seydou, F. Maurel, B. TANGOUR, Intramolecular Path Determination of Active Electrons on Push-Pull Oligocarbazole Dyes-Sensitized Solar Cells, ChemistryOpen 8 (2019) 580–588.
[69] N. Kouki, S. Trabelsi, M. Seydou, F. Maurel, B. TANGOUR, Internal path investigation of the acting electrons during the photocatalysis of panchromatic ruthenium dyes in dye-sensitized solar cells, Comptes Rendus Chimie 22 (2019) 34–45.
[70] R. Bessrour, Y. Belmiloud, Z. Hosni, B. Tangour, Controlling drug efficiency by encapsulation into carbon nanotubes: A theoretical study of the antitumor Cisplatin and the anti-HIV TIBO molecules, Pavia, Italy, 2012, pp. 229–239.
[71] Z. Hosni, R. Bessrour, B. TANGOUR, 195Pt Chemical Shift Ability to Control the Antitumor Drug Cisplatin Encapsulated Into Carbon Nanotubes: A Theoretical Study, j comput theor nanosci 11 (2014) 318–323.
[72] A. MEJRI, B. TANGOUR, G. Herlem, F. Picaud, Confinement of the antitumoral drug cisplatin inside edge-functionalized carbon nanotubes and its release near lipid membrane, Eur. Phys. J. D 75 (2021).

[73] A. MEJRI, D. Vardanega, B. TANGOUR, T. Gharbi, F. Picaud, Encapsulation into carbon nanotubes and release of anticancer Cisplatin drug molecule, The journal of physical chemistry. B 119 (2015) 604–611.
[74] Y. Belmiloud, M. Ouraghi, M. Brahimi, A. Benaboura, D. Charqaoui, B. Tangour, Theoretical Study of the Anti-Human Immuno-Deficiency Virus TIBO Molecule Confined Into Carbon Nanotubes, j comput theor nanosci 9 (2012) 1101–1108.
[75] M. Mlaouah, B. TANGOUR, M. El Khalifi, T. Gharbi, F. Picaud, The encapsulation of the gemcitabine anticancer drug into grapheme nest: a theoretical study, Journal of molecular modeling 24 (2018) 102.
[76] H. Khemir, B. TANGOUR, F. Moussa, An " In Silico " Study of Drug Vectorization by a Carbon Nanocone, j comput theor nanosci 13 (2016) 3384–3392.
[77] H. Besrour, B. TANGOUR, R. Linguerri, M. Hochlaf, Encapsulation of anticancer drug doxorubicin inside dendritic macromolecular cavities: First-principles benchmarks, Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy 217 (2019) 278–287.