

## CURRICULUM VITAE

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1 November 2021



### Contact Information

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### Present Status:

Assistant Professor of Inorganic Chemistry

### Education:

**Ph.D (Inorganic Chemistry):** Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran (2009 to 2014)

**Title:** Syntheses, theoretical, spectroscopic and structural studies of new phosphoramidates having the C(O)NHP(O) and P(O)(N<sup>1</sup>)(N<sup>2</sup>)(N<sup>3</sup>) skeletons and their using as oxygen donor ligands in preparation of new complexes

**M.Sc. (Inorganic Chemistry):** Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran (2007 to 2009)

**Title:** Theoretical studies on polyoxometalate compounds with the formula [PdV<sub>6</sub>O<sub>18</sub>]<sup>4-</sup> and [Mo<sub>7</sub>O<sub>16</sub>(O<sub>3</sub>PCH<sub>2</sub>PO<sub>3</sub>)<sub>3</sub>]<sup>9-</sup>

**B.Sc. (Pure Chemistry):** Department of Chemistry, Faculty of Sciences, Shiraz University, Shiraz, Iran (2002 to 2006)

**Teaching Experience:**

**For Undergraduate:**

1. General Chemistry
2. Inorganic Chemistry I, II & III
3. Inorganic Chemistry Lab. I & II

**For Graduate:**

1. Advanced Inorganic Chemistry
2. Metal Organic Chemistry
3. Recent Topics in Inorganic Chemistry
4. Crystallography
5. Computational Chemistry

**Research Interests:**

1. Synthesis of New Phosphoramides and their coordination compounds.
2. Crystal Structure and CSD analysis of Phosphoramides and their coordination compounds.
3. Synthesis and Spectroscopic study (IR, NMR and Mass) of New Phosphorus-Nitrogen compounds and their Coordination Chemistry.
4. Computational Analysis on Inorganic Compounds.
5. Synthesis of New Inorganic Nano-structures.
6. Biological Analysis on Inorganic Compounds

**List of Publication:**

1. Synthesis and structural study of five new phosphoric triamides: interplay between classical and non-classical intermolecular interactions,

Bahar Bakhshipour, Atekeh Tarahhomi, Arie van der Lee, *Z. Kristallogr.* (2021) 236: 282 – 294.

2. Coordination versus hydrogen bonds in the structures of different tris(pyridin-2-yl)phosphoric triamide derivatives,

Marjan Sebghati, **Atekeh Tarahhomi**, Marjan Sadat Bozorgvar, Dan G. Dumitrescu, Arie van der Lee, *RSC Adv.* (2021) 11:8178.

3. Synthesis and structural study of two new phosphorus-oxygen compounds belonging to two different families of phosphoramides and phosphates,

Marjan Sadat Bozorgvar, **Atekeh Tarahhomi**, A Van Der Lee, *J. Applied Chem.* (2021) 16:, 95-106.

4. Structural studies on two new phosphoramides with the same [OC 4 H 8 N]P(O) segment by means of single-crystal X-ray diffraction, Hirshfeld surface analysis and 3D energy framework approach,

Marjan Sadat Bozorgvar, **Atekeh Tarahhomi**, Arie van der Lee, *J. Mol. Struct.* (2020) 1223: 128942.

5. Evaluation of structural, spectroscopic, bonding and electronic properties of some organotin(IV)-phosphoric triamide complexes by using help of DFT, QTAIM and Hirshfeld surface investigations,

Raheleh Fallah baneh kohal, **Atekeh Tarahhomi**, *Comput. Theor. Chem.* (2021) 1195:113098.

6. Association of Non-covalent Interactions C—H...X (X=O, F, Cl,  $\pi$ ) and Cl... $\pi$  with Hydrogen Bond Interactions N—H...O in Molecular Assembly of New Phosphoramides: A Combined X-Ray Crystallography and Topology (AIM and Hirshfeld) Analysis,

Marjan Sebghati, **Atekeh Tarahhomi**, Anna Kozakiewicz, *ChemistrySelect* (2020) 5: 185 – 195.

7. Three new amidophosphoric acid esters with a P(O)[OCH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>O] segment: X-ray diffraction, DFT, AIM and Hirshfeld surface investigations of bi- and tri-furcated (three and four-center) hydrogen bond interactions,

Marjan Sadat Bozorgvar, **Atekeh Tarahhomi**, Arie van der Lee, *Z. Kristallogr.* (2020) 235: 69 – 84.

8. Evaluation of N—H...O hydrogen bond interactions in two new phosphoric triamides with a P(O)[NHCH(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub> segment by means of topological (AIM) calculations, Hirshfeld surface analysis and 3D energy framework approach

**Atekeh Tarahhomi**, Arie van der Lee, Dan G. Dumitrescu, *Z. Kristallogr.* (2019) 234: 401 – 413.

9. A detailed theoretical and experimental study on the N—H, P=O and C=O stretching frequencies in two new phosphoric triamides and a statistical comparison with analogous structures

**Atekeh Tarahhomi**, Arie van der Lee, Borys Ośmiałowski, *Polyhedron* (2019) 158: 215 – 224.

10. Synthesis and crystal structures of new phosphoric triamides: study of intermolecular interactions by semi-empirical calculations and Hirshfeld surface analysis

**Atekeh Tarahhomi**, Arie van der Lee, *Monatsh Chem.* (2018) 149: 1759 – 1776.

**11.** A new six-coordinate organotin(IV) complex of OP[NC<sub>5</sub>H<sub>10</sub>]<sub>3</sub>: A comparison with an analogous five-coordinate complex by means of X-ray crystallography, Hirshfeld surface analysis and DFT calculations

**Atekeh Tarahhomi**, Arie van der Lee, *J. Coord. Chem.* (2018) 71: 1575 – 1592.

**12.** Synthesis, crystal structure and Hirshfeld surface analysis of new phosphoric triamide [2-F-C<sub>6</sub>H<sub>4</sub>C(O)NH]P(O)[NHCH(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub>,

**Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *J. Appl. Chem.* (2017) 11: 23 – 30.

**13.** Synthesis and characterization of two new phosphoric triamides: structural study of OP[NHC<sub>5</sub>H<sub>9</sub>]<sub>3</sub>

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, Arnold L. Rheingold, James A. Golen, *J. Appl. Chem.* (2017) 12: 243 – 252.

**14.** A new Z' = (2 + 0.5 + 0.5) amidophosphoester structure: Hirshfeld surface analysis of symmetry-independent molecules,

Mojtaba Keikh, Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arie van der Lee, *Z. Kristallogr.* (2017) 232: 453 – 462.

**15.** The first coordination compounds of OP[NC<sub>4</sub>H<sub>8</sub>O]<sub>3</sub> phosphoric triamide ligand: structural study and Hirshfeld surface analysis of Sn<sup>IV</sup> and Mn<sup>II</sup> complexes,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, James A. Golen & Arnold L. Rheingold, *J. Coord. Chem.* (2017) 70: 1285 – 1302.

**16.** Crystal structures, DFT calculations, and Hirshfeld surface analyses of two new copper(II) and nickel(II) Schiff base complexes derived from meso-1,2-diphenyl-1,2-ethylenediamine,

Leila Seifikar Ghomi, Mahdi Behzad, **Atekeh Tarahhomi**, Ali Arab, *J. Mol. Struct.* (2017) 1150: 214 – 226.

**17.** Syntheses and structures of four new mixed-amide phosphoric triamides,

Mojtaba Keikh, Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arie van der Lee, *Acta Cryst. Section C* (2016) C72: 251 – 259.

**18.** Crystal structures, DFT calculations and Hirshfeld surface analyses of three new cobalt(III) Schiff base complexes derived from meso-1,2-diphenyl-1,2-ethylenediamine,

Mohaddeseh Masoudi, Mahdi Behzad, Ali Arab, **Atekeh Tarahhomi**, Hadi Amiri Rudbari, Giuseppe Bruno, *J. Mol. Struct.* (2016) 1122: 123 – 133.

**19.** Synthesis, crystal structures and Hirshfeld surface analyses of two new Salen type nickel/sodium heteronuclear complexes,

Niloofer Mahlooji, Mahdi Behzad, **Atekeh Tarahhomi**, Michael Maroney, Hadi Amiri Rudbari, Giuseppe Bruno, Bahram Ghanbari, *J. Mol. Struct.* (2016) 1110:119 – 127.

**20.** Three new phosphoric triamides with a  $[\text{C}(\text{O})\text{NH}]\text{P}(\text{O})[\text{N}(\text{C})(\text{C})]_2$  skeleton: a database analysis of C—N—C and P—N—C bond angles,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section C*, (2014) 70:998 – 1002.

**21.** Hirshfeld surface analysis of the 1,1'-(ethane-1,2-diyl) dipyridinium dication in two new salts: perchlorate and peroxydisulfate,

Mostafa Gholizadeh, Mehrdad Pourayoubi, Masoumeh Farimaneh, **Atekeh Tarahhomi**, Michal Dušek, Václav Eigner *Acta Crystallogr. Section C*, (2014) 70:230 – 235.

**22.** Hirshfeld surface analysis of new organotin (IV)-phosphoramidate complexes,

Mehrdad Pourayoubi, Samad Shoghpor Bayraq, **Atekeh Tarahhomi**, Marek Nečas, Karla Fejfarová, Michal Dušek, *J. Organomet. Chem.* (2014) 751:508 – 518.

**23.** Hirshfeld surface analysis of new phosphoramidates,

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, James A Golen, Poorya Zargaran, Behrouz Elahi, Arnold L Rheingold, Leyva Ramírez, Teresa Mancilla Percino, *Acta Crystallogr. Section B*, (2013) 69:260 – 270.

**24.** Two new  $\text{XP}(\text{O})[\text{NHC}(\text{CH}_3)_3]_2$  phosphoramidates, with  $X = (\text{CH}_3)_2\text{N}$  and  $[(\text{CH}_3)_3\text{CNH}]_2\text{P}(\text{O})(\text{O})$ . Corrigendum,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Fatemeh Karimi Ahmadabad, Karla Fejfarová, Arie van der, Michal Dušek, *Acta Crystallogr. Section C*, (2013) 69:453.

**25.** A novel amido–pyrophosphate  $\text{Mn}^{\text{II}}$  chelate complex with the synthetic ligand  $\text{O}\{\text{P}(\text{O})[\text{NHC}(\text{CH}_3)_3]_2\}_2$  (*L*):  $[\text{Mn}(\text{L})_2\{\text{OC}(\text{H})\text{N}(\text{CH}_3)_2\}_2]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ ,

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, Karla Fejfarová, Michal Dušek, *Acta Crystallogr. Section C*, (2013) 69: 225 – 228.

**26.** *N*-(4-Fluorobenzoyl)-*N',N''*-diisopropylphosphoric triamide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section C*, (2012) 68:o3406 – o3407.

**27.** *N,N,N',N''*-Tetrabenzyl-*N''*-(2, 6-difluorobenzoyl) phosphoric triamide,

A Raissi Shabari, Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L Rheingold, James A Golen, *Acta Crystallogr. Section E*, (2012) 68:o3186-o3186.

**28.** A second monoclinic polymorph of *N*-[bis(morpholin-4-yl)phosphinoyl]-4-fluorobenzamide with the  $P2_1/n$  space group,

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, Mojtaba Keikha, Arnold L Rheingold, James A Golen, *Acta Crystallogr. Section E*, (2012) 68:o2444.

**29.** Crystal structure of *N,N,N',N''*-tetrakis(4-methylphenyl)-diphosphoric tetra-amide,  $C_{28}H_{32}N_4O_3P_2$ ,

Mehrdad Pourayoubi, Hassan Fadaei, **Atekeh Tarahhomi**, Masood Parvez, *Z. Kristallogr.-New Crystal Structures*, (2012) 227:205 – 206.

**30.** Phosphoramidates: Molecular Packing and Hydrogen Bond Strength in Compounds Having a  $P(O)(N)_n(O)_{3-n}$  ( $n= 1, 2, 3$ ) Skeleton,

Mehrdad Pourayoubi, Fahimeh Sabbaghi, Vladimir Divjakovic, **Atekeh Tarahhomi**, *Advances in Crystallization Processes* (2012) IntechOpen.

**31.** *O*-Phenyl (tert-butylamido)(*p*-tolylamido) phosphinate,

Mehrdad Pourayoubi, Arnold L Rheingold, Chao Chen, F Karimi Ahmadabad, **Atekeh Tarahhomi**, *Acta Crystallogr. Section E*, (2012) 67:o3405 – o3406.

**32.** *N,N'*-Dicyclohexyl-*N''*-(2,6-difluorobenzoyl)-*N,N'*-dimethylphosphoric triamide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2012) 67:o3027.

**33.** *N,N,N',N'*-Tetraethyl-*N''*-(2-fluorobenzoyl)phosphoric triamide,

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2011) 67:o2643.

**34.** Cyclohexyl (methyl) ammonium {bis[cyclohexyl(methyl)amino] phosphoryl}(4-methylphenylsulfonyl) azanide,

Mehrdad Pourayoubi, Hassan Fadaei, **Atekeh Tarahhomi**, Masood Parvez, *Acta Crystallogr. Section E*, (2011) 67:o2795.

**35.** *N*-(2,6-Difluorobenzoyl)-*P,P*-bis(pyrrolidin-1-yl) phosphinic amide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2012) 67:o2444.

**36.** Different cyclic motifs in phosphoric triamides containing a  $C(O)NHP(O)(NH)_2$  skeleton and an  $R_2^2(10)$  graph set in three new compounds: a database analysis of hydrogen-bond strengths based on motifs,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Anahid Saneei, Arnold L Rheingold, James A Golen, *Acta Crystallogr. Section C*, (2011) 67:o265 – o272.

**37.** *N*-(2-Fluorobenzoyl)-*N',N''*-bis (4-methylphenyl) phosphoric triamide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2011) 67:o934.

**38.** Different orientations of C=O versus P=O in P(O)NHC(O) skeleton: the first study on an aliphatic diazaphosphorinane with a *gauche* orientation,

**Atekeh Tarahhomi**, Mehrdad Pourayoubi, Arnold L. Rheingold, James A. Golen., *Struct. Chem.* (2011) 22:201-210.

**39.** *N,N'*-Di-tert-butyl-*N''*-(2,6-difluorobenzoyl) phosphoric triamide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2010) 66:o3159.

**40.** *N,N'*-Dibenzyl-*N''*-(2,6-difluorobenzoyl)-*N,N'*-dimethylphosphoric triamide,

Mehrdad Pourayoubi, **Atekeh Tarahhomi**, Arnold L. Rheingold, James A. Golen, *Acta Crystallogr. Section E*, (2010) 66:o2524.

## Papers Presented at Conferences and Seminars

**1.** Hirshfeld surface analysis of co-crystal  $\text{P(O)(NHC}_6\text{H}_{11})_3(\text{C}_6\text{H}_{11}\text{NH}_3)^+(\text{CH}_3\text{COO})^-$  and proton transfer  $[\text{C}_6\text{H}_{11}\text{NH}_2\text{CH}_3]^+[\text{4-CH}_3\text{C}_6\text{H}_4\text{S(O)}_2\text{NP(O)[N(CH}_3\text{)(C}_6\text{H}_{11})_2}]^-$ ,

*Atekeh Tarahhomi, 19th Iranian Seminar of Chemistry, Shiraz, Shiraz University, Iran 2017.*

**2.** New Organotin (IV)-Phosphoramidate Complex: *Cis*-Dichlorido-*Trans*-Dimethyl-*Cis*-Bis(*N,N',N''*-Tricyclopentylphosphoric Triamide) Tin (IV),

*Atekeh Tarahhomi, Mehrdad Pourayoubi, 14th Iranian Inorganic Chemistry Conference, Sharif University of Technology, Tehran, Iran, 28-29 August, 2012.*

**3.** Synthesis and crystal structure of *N*-(2-fluorobenzoyl)-*N',N'*-diisopropylphosphoric triamide,

*Atekeh Tarahhomi, Mehrdad Pourayoubi, 15th Iranian Chemistry Conference, Bu-Ali Sina University, Hamedan, Iran, 2011.*

**4.** Crystal structure and H-bond pattern of a new acetyl phosphorylamidate,

*Atekeh Tarahhomi, Mehrdad Pourayoubi, 15th Iranian Chemistry Conference, Bu-Ali Sina University, Hamedan, Iran, 2011.*

**5.** Crystal structure, hydrogen bonds and C—X... $\pi$  (X= H, F) interactions of a new acetyl phosphorylamidate,

Atekeh Tarahhomi, Mehrdad Pourayoubi, *12th Iranian Inorganic Chemistry Conference (2010)*.