A New 1D Ni (II) Coordination Polymer of *s*-Triazine Type Ligand and Thiocyanate as Linker via Unexpected Hydrolysis of 2,4-*bis*(3,5-dimethyl-*1H*-pyrazol-1-yl)-6-methoxy-1,3,5-triazine

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Physicochemical characterizations

FTIR spectra were recorded using Alpha Bruker spectrophotometer. The CHNS analyses were performed on a Perkin-Elmer 2400 elemental analyzer. The Ni content was determined using Shimadzu atomic absorption spectrophotometer (AA-7000 series, Shimadzu, Ltd, Japan). All chemicals were purchased from Aldrich Company.

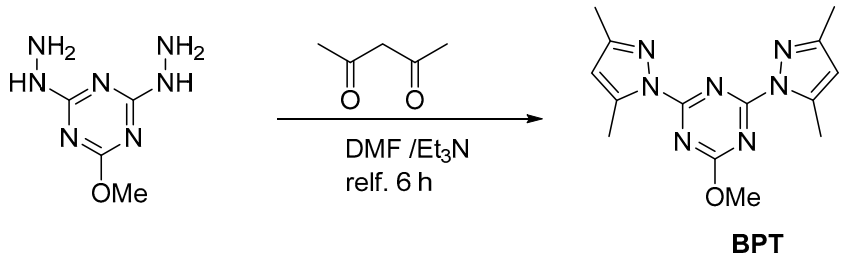
X-ray measurements

The crystal of $[Ni(MPT)(H_2O)(SCN)_2]_n$ was and measured at a temperature of 289 K. The X-ray diffraction data was collected on a Bruker Apex-II CCD diffractometer using Mo Kα radiation. The APEX2/SAINT [63] software package was used for cell refinement and data reduction. A multi-scan absorption correction (SADABS [64]) was applied to the intensities before structure solution. Structure was solved by direct methods with SHELXS-97 [65] software. Structural refinement was carried out using SHELXL-2019/2 [66] software with SHELXLE [67] graphical user interface. The crystal under investigation contains solvent of crystallization. Most likely there are both CH_3OH and H_2O molecules in the structure. However, the solvent molecules are partially lost and disordered. Therefore, the solvent of crystallization could not be unambiguously determined and was omitted from the final refinement cycles. The contribution of the missing solvent to the calculated structure factors was taken into account by using the SQUEEZE routine of PLATON [68]. The contribution of the missing solvent to the unit cell content was not taken into account. H_2O and O-H hydrogen atoms were placed on idelized position with O-H distances of 0.86 Å and O-H = 0.82 Å respectively and with U_{iso} = 1.5 U_{eq} (parent atom). Other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95-0.98 Å and U_{iso} = 1.2-1.5 U_{eq} (parent atom). The highest peak is located 0.79 Å from atom Ni1 and the deepest hole is located 0.94 Å from atom S1.

Method S1: Synthesis of BPT

At room temperature, 2,4-dihydrazinyl-6-methoxy-1,3,5-triazine (10 mmol in 20 mL DMF) was mixed with acetylacetone (25 mmol) followed by addition of triethylamine (8 mmol in 10 mL DMF) with stirring then refluxed for 6 h (**Scheme 1)**. After completion of the reaction, the mixture is left to cool till room temperature, and then ice-cold water was added (100 mL). The reaction mixture was kept at 0^{o}C for 2 h, white solid powder of **BPT** is precipitated. The product is filtered, washed with cold water (3 x 20 mL), and then dried.

Yield; $C_{14}N_7H_{17}O$ (**BPT**) 86%; mp 175-176 °C. Anal. Calc. C, 56.18; H, 5.72; N, 32.76%. Found: C, 56.16; H, 5.74; N, 32.77%; IR (KBr, cm^{-1}): 3041, 2978, 2926, 1593, 1555; (**Fig. S2**, Supplementary data). ^{1}H NMR ($CDCl_3$) δ: 2.30 (s, 6H, $2CH_3$), 2.72 (s, 6H, $2CH_3$), 4.12 (s, 3H, OCH_3),6.05 (s, 2H, CH) ppm (**Fig. S3**, Supplementary data); ^{13}C NMR ($CDCl_3$): δ 13.8, 17.8, 55.7, 111.9, 144.4, 153.3, 164.8, 172.3 ppm (**Fig. S3**, Supplementary data).



Scheme S1: Synthesis of the ligand (**BPT**).

Method S2: Biological studies

Evaluation of Cytotoxic Effects

Mammalian cell lines: HepG-2 cells (human Hepatocellular carcinoma) and **A-549** cells (human Lung cancer cell line) were obtained from VACSERA Tissue Culture Unit.

Chemicals Used: Dimethyl sulfoxide (DMSO), crystal violet and trypan blue dye were purchased from Sigma (St. Louis, Mo., USA). Fetal Bovine serum, DMEM, RPMI-1640, HEPES buffer solution, L-glutamine, gentamycin and 0.25% Trypsin-EDTA were purchased from Lonza.

Crystal violet stain (1%): It composed of 0.5% (w/v) crystal violet and 50% methanol then made up to volume with ddH_2O and filtered through a Whatmann No.1 filter paper.

Cell line Propagation:

The cells were propagated in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% heat-inactivated fetal bovine serum, 1% L-glutamine, HEPES buffer and 50μg/ml gentamycin. All cells were maintained at 37ºC in a humidified atmosphere with 5% CO_2 and were subcultured two times a week.

Cytotoxicity evaluation using viability assay: For cytotoxicity assay, the cells were seeded in 96-well plate at a cell concentration of 1×10^4 cells per well in 100μl of growth medium. Fresh medium containing different concentrations of the test sample was added after 24 h of seeding. Serial two-fold dilutions of the tested chemical compound were added to confluent cell monolayers dispensed into 96-well, flat-bottomed microtiter plates (Falcon, NJ, USA) using a multichannel pipette. The microtiter plates were incubated at 37ºC in a humidified incubator with 5% CO_2 for a period of 24 h. Three wells were used for each concentration of the test sample. Control cells were incubated without test sample and with or without DMSO. The little percentage of DMSO present in the wells (maximal 0.1%) was found not to affect the experiment. After incubation of the cells for at 37°C, for 24 h, the viable cells yield was determined by a colorimetric method.

In brief, after the end of the incubation period, media were aspirated and the crystal violet solution (1%) was added to each well for at least 30 minutes. The stain was removed and the plates were rinsed using tap water until all excess stain is removed. Glacial acetic acid (30%) was then added to all wells and mixed thoroughly, and then the absorbance of the plates were measured after gently shaken on Microplate reader (TECAN, Inc.), using a test wavelength of 490 nm. All results were corrected for background absorbance detected in wells without added stain. Treated samples were compared with the cell control in the absence of the tested compounds. All experiments were carried out in triplicate. The cell cytotoxic effect of each tested compound was calculated**.** The optical density was measured with the microplate reader (SunRise, TECAN, Inc, USA) to determine the number of viable cells and the percentage of viability was calculated as [(ODt/ODc)]x100% where ODt is the mean optical density of wells treated with the tested sample and ODc is the mean optical density of untreated cells. The relation between surviving cells and drug concentration is plotted to get the survival curve of each tumor cell line after treatment with the specified compound. The 50% inhibitory concentration (IC_{50}), the concentration required to cause toxic effects in 50% of intact cells, was estimated from graphic plots of the dose response curve for each conc. using Graphpad Prism software (San Diego, CA. USA).

Evaluation of Cytotoxic Effects of certain Chemical compound

Mammalian cell lines: WI-38 cells (human lung fibroblast normal cells), were obtained from the American Type Culture Collection (ATCC, Rockville, MD).

Chemicals Used: Dimethyl sulfoxide (DMSO), crystal violet and trypan blue dye were purchased from Sigma (St. Louis, Mo., USA).

Fetal Bovine serum, DMEM, RPMI-1640, HEPES buffer solution, L-glutamine, gentamycin and 0.25% Trypsin-EDTA were purchased from Lonza.

Crystal violet stain (1%): It composed of 0.5% (w/v) crystal violet and 50% methanol then made up to volume with ddH_2O and filtered through a Whatmann No.1 filter paper.

Cell line Propagation:

The cells were propagated in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% heat-inactivated fetal bovine serum, 1% L-glutamine, HEPES buffer and 50µg/ml gentamycin. All cells were maintained at 37ºC in a humidified atmosphere with 5% CO_2 and were subcultured two times a week.

Cytotoxicity evaluation using viability assay: For cytotoxicity assay, the cells were seeded in 96-well plate at a cell concentration of 1×10^4 cells per well in 100µl of growth medium. Fresh medium containing different concentrations of the test sample was added after 24 h of seeding. Serial two-fold dilutions of the tested chemical compound were added to confluent cell monolayers dispensed into 96-well, flat-bottomed microtiter plates (Falcon, NJ, USA) using a multichannel pipette. The microtiter plates were incubated at 37ºC in a humidified incubator with 5% CO_2 for a period of 24 h. Three wells were used for each concentration of the test sample. Control cells were incubated without test sample and with or without DMSO. The little percentage of DMSO present in the wells (maximal 0.1%) was found not to affect the experiment. After incubation of the cells viable cells yield was determined by a colorimetric method.

In brief, after the end of the incubation period, media were aspirated and the crystal violet solution (1%) was added to each well for at least 30 minutes. The stain was removed and the plates were rinsed using tap water until all excess stain is removed. Glacial acetic acid (30%) was then added to all wells and mixed thoroughly, and then the absorbance of the plates were measured after gently shaken on Microplate reader (TECAN, Inc.), using a test wavelength of 490 nm. All results were corrected for background absorbance detected in wells without added stain. Treated samples were compared with the cell control in the absence of the tested compounds. All experiments were carried out in triplicate. The cell cytotoxic effect of each tested compound was calculated**.** The optical density was measured with the microplate reader (SunRise, TECAN, Inc, USA) to determine the number of viable cells and the percentage of viability was calculated as [(ODt/ODc)]x100% where ODt is the mean optical density of wells treated with the tested sample and ODc is the mean optical density of untreated cells. The relation between surviving cells and drug concentration is plotted to get the survival curve of each tumor cell line after treatment with the specified compound. The Cytotoxic concentration (CC_{50}), the concentration

required to cause toxic effects in 50% of intact cells, was estimated from graphic plots of the dose response curve for each conc. using Graphpad Prism software (San Diego, CA. USA).

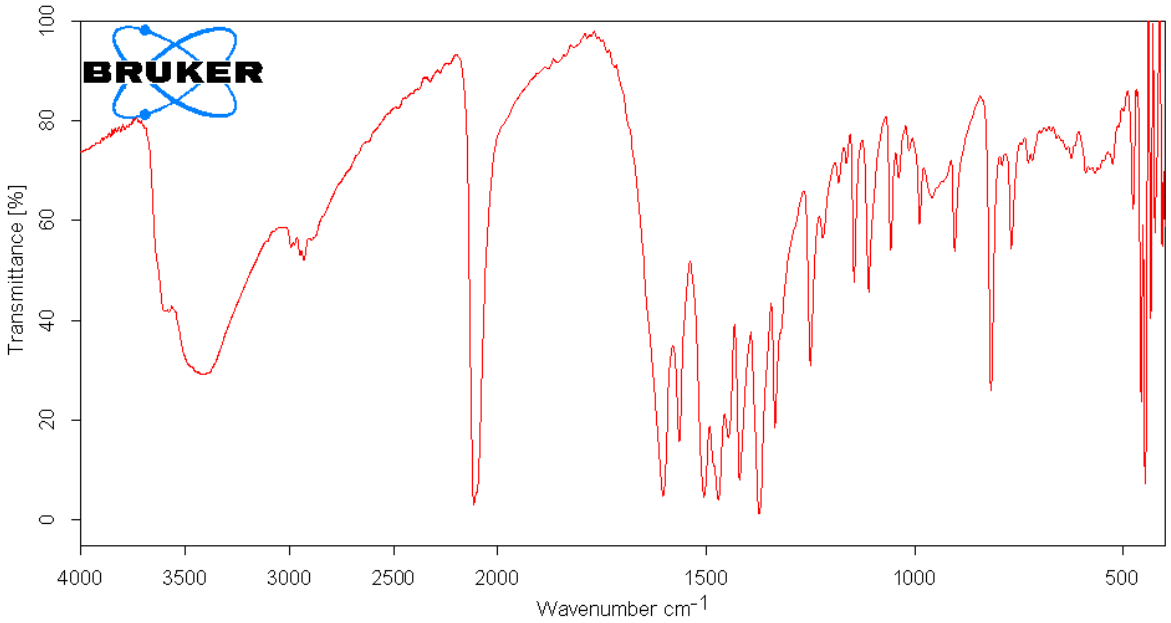


Figure S1: FTIR spectra of $[Ni(MPT)(H_2O)(SCN)_2]_n$ complex.

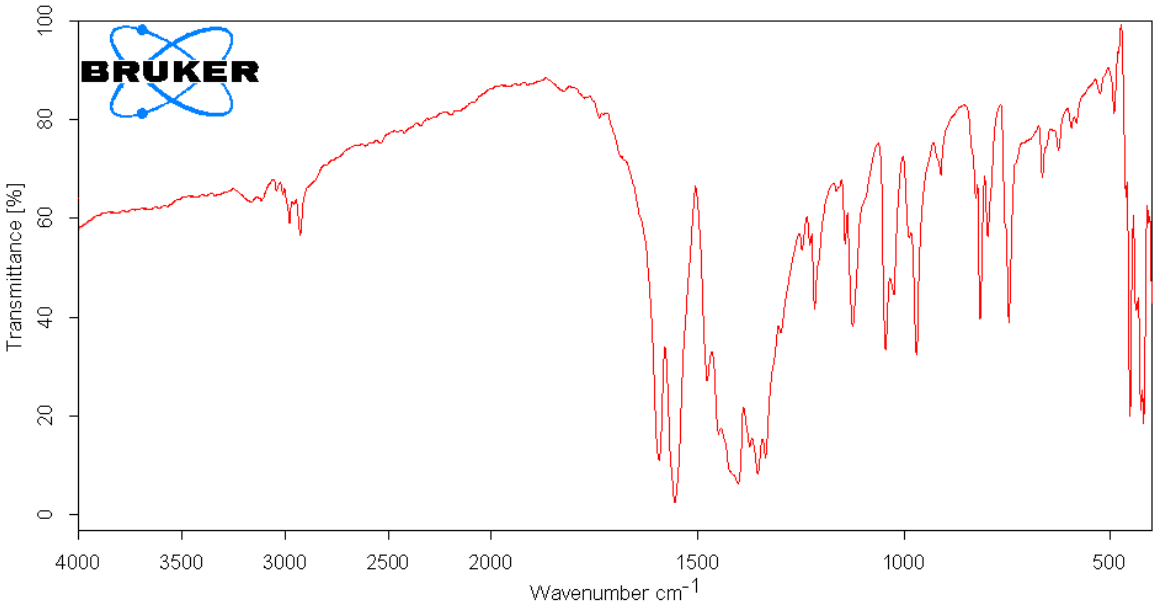
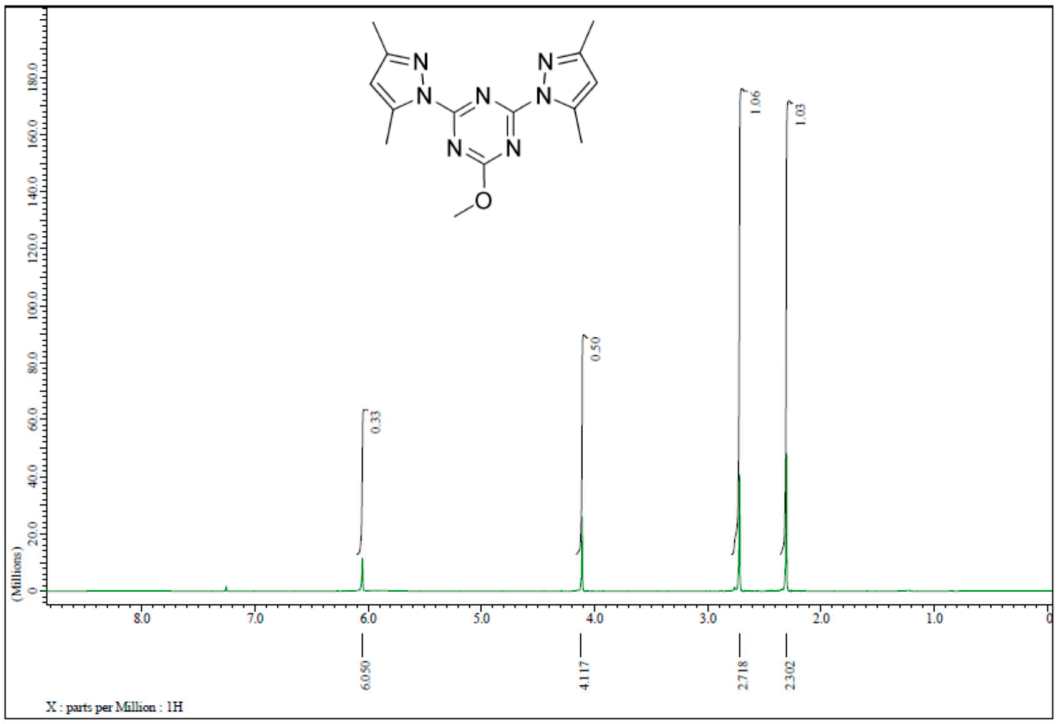


Figure S2: FTIR spectra of BPT ligand.



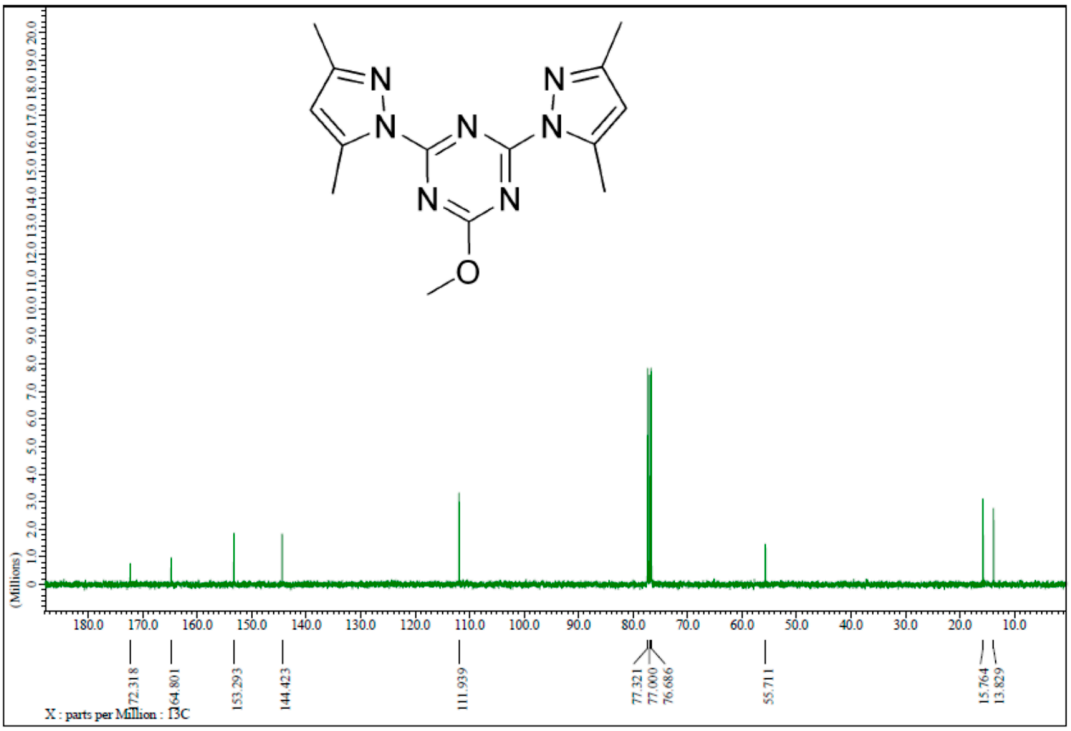


Figure S3: ^{1}H and ^{13}C NMR spectra of the ligand (**BPT**). Chemical shifts are reported in parts per million (ppm).

Table S1: The cytotoxicity of the studied complex against HepG-2 cell line

Sample conc. (µg/mL)	Viability %	Inhibitory %	S.D. (±)
500	5.42	94.58	0.54
250	13.89	86.11	0.63
125	28.65	71.35	1.79
62.5	43.81	56.19	2.07
31.25	69.40	30.6	2.34
15.6	85.12	14.88	1.66
7.8	97.43	2.57	0.95
3.9	100	0	
2	100	0	
1	100	0	
0	100	0	

Table S2: The cytotoxicity of the studied complex against A-549 cell line

Sample conc. (µg/mL)	Viability %	Inhibitory %	S.D. (±)
500	6.76	93.24	0.82
250	19.47	80.53	0.69
125	35.84	64.16	1.92
62.5	48.19	51.81	2.43
31.25	82.86	17.14	2.78
15.6	98.41	1.59	0.65
7.8	100	0	
3.9	100	0	
2	100	0	
1	100	0	
0	100	0	