# A series of transitional metal coordination polymers based on a rigid bi-functional carboxylate-triazolate tecton

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## 1. Introduction of Genetic Algorithm-Quantum Monte Carlo (GA-QMC) program
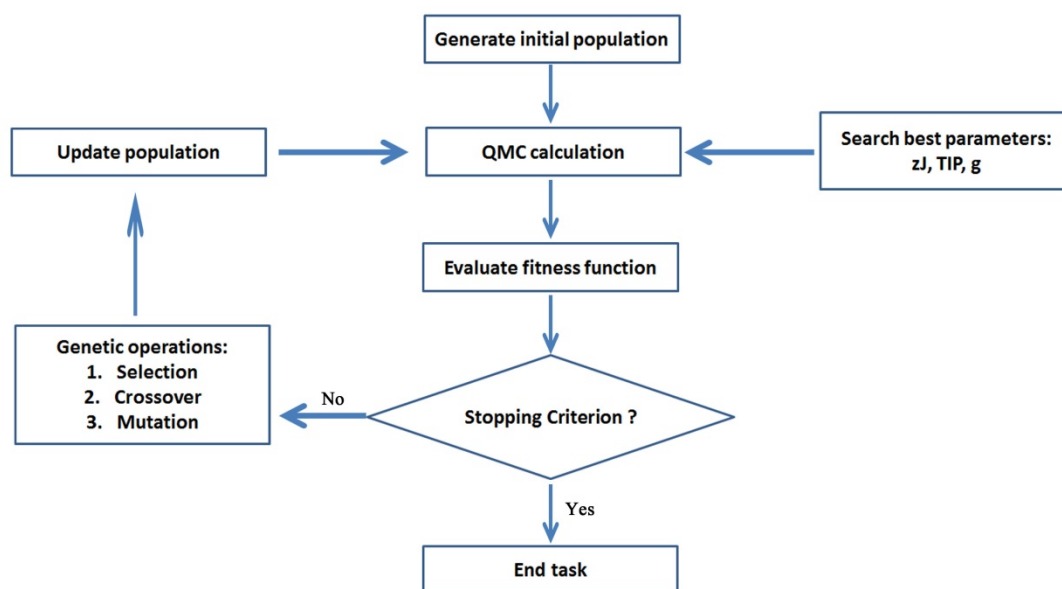


Figure S1 running procedure of GA-QMC programs.

**Genetic Algorithm details of GA-QMC:**

Genetic Algorithm ( GA ) found by Holland[1] is an adaptive heuristic search algorithm based on the evolutionary ideas of natural selection and genetics. It features the genetic structure and behaviour of chromosomes within a population of individuals. Thus, GA becomes an effective tool in searching a large state-space, multi-modal state-space, or n-dimensional surface. In this program, GA contains following steps:

1. According to the constraint of coupling parameters ( $J_1$ and $J_2$), one initial population, consisting of a certain number of chromosomes, were generated

randomly by using of binary encoding. In this simulation, population size was set to 30.

2. All of chromosomes in current population are decoded successively and further conducted QMC simulation. For each QMC simulation, zJ, TIP and g factor were obtained by exhaustive method, and the optimal reliability factors ( R ) were converted into fitness values based on following formula:

$$Fitness = \begin{cases} c - R, & if \ R < c \\ 0 & Otherwise \end{cases}$$

In this simulation, $c$ constant is set to 1.0. We also changed the value of c constants to 1.0 or 0.01, and found that the value cannot affect finial results.

3. Judge stopping criterion. If total running generations is equal to setting value, simulation will be over. If not, continue to 4th step.

4. Conduct three genetic operations:

   4.1 **Selection**: Both roulette wheel method and elite-individual preservation law are used to produce offspring. In order to keep offspring diversity on the propagation of parent, repetition number of new individual was restrained to less than **5**. This strategy can avoid the simulation to involve local stable state.

   4.2 **Crossover**: Two-point crossover method is utilized in this simulation. Crossover probability ( $P_c$ ) is set to 0.45.

   4.3 **Mutation**: Each gene mutation is dominated by mutation probability ( $P_m$ ). In this simulation, $P_m$ is set to 0.015.

5. Update new population, and return to perform the 2nd step.

**QMC Simulation Detail**:

Quantum Monte Carlo module were written based on LOOP[2] of ALPS library [3]. Specifically, three parameters ($g$, $zJ$ and $TIP$ ) were further used to fit experimental M-T curve by use of exhaustive-iterative method. The corresponding formulas were shown in Eq(1)-Eq(4). Until the running is over, the best parameters ($R_b$, $g_b$, $TIP_b$, $zJ_b$) were obtained. The detailed MC parameters are presented as follows: For each site, $2 \times 10^6$ Monte Carlo Steps (MCS) and 10%

MCS for thermalization were performed. The spins sample of 400 for **1-Cu** and 200 for **2-Mn** is large enough to prevent any finite size effects. Moreover, periodic boundary conditions (PBC) were applied in order to avoid perturbation from the edge of the sample and speed up convergence toward the infinite lattice limit.

$$\chi_u = \frac{1}{NT} \left\langle \left( \sum_{i=1}^{N} S_i^z \right)^2 \right\rangle$$

Eq(1)

where uniform magnetic susceptibility $\chi_u$ is dimensionless.

Convert uniform magnetic susceptibility to $\chi_T$ ($cm^3 mol^{-1}$)

$$\chi_T (cm^3 mol^{-1}) = Ag^2 \chi_u$$

Eq(2)

where $g$ is Landé $g$-factor and $A$ is unit constant.

Import $zJ$ and $TIP$ factor to $\chi_T$, as bellows:

$$\chi_T' (cm^3 mol^{-1}) = \frac{(\chi_T + TIP)}{1 + \frac{zJ(\chi_T + TIP)}{0.1303g^2}}$$

Eq(3)

The reliability factor $R$ is obtained by

$$R = \frac{\sum (\chi_T' T - \chi_{obs} T)^2}{\sum (\chi_{obs} T)^2}$$

Eq(4)

**Note**: GA-QMC program was written by using of C++ language and compiled by using of Intel C++ ( version 14.0.2 ). Random number of GA code was obtained by using random number generator of Intel Math Kernel Library ( MKL ). Following Message-Passing Interface ( MPI ) standard, parallel program was written by using of MPICH 2.0. All GA-QMC calculations were conducted on 4 twelve-cores nodes of in the National Shenzhen Supercomputing center of china. The evolution of R value was presented in Fig. S2.
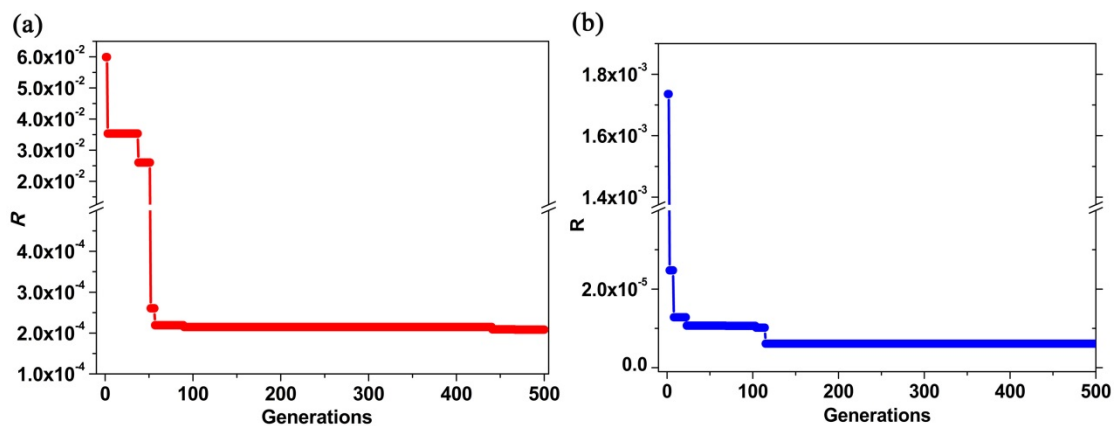
Figure S2 the changes of R values with genetic evolution: (a) 1-Cu; (b) 2-Mn.

Reference:

[1] J. H. Holland, Adaptation in natural and artificial system, Ann Arbor, The University of Michigan Press, 1975.

[2] S. Todo and K. Kato, *Phys. Rev. Lett.*, 2001, 87, 047203.

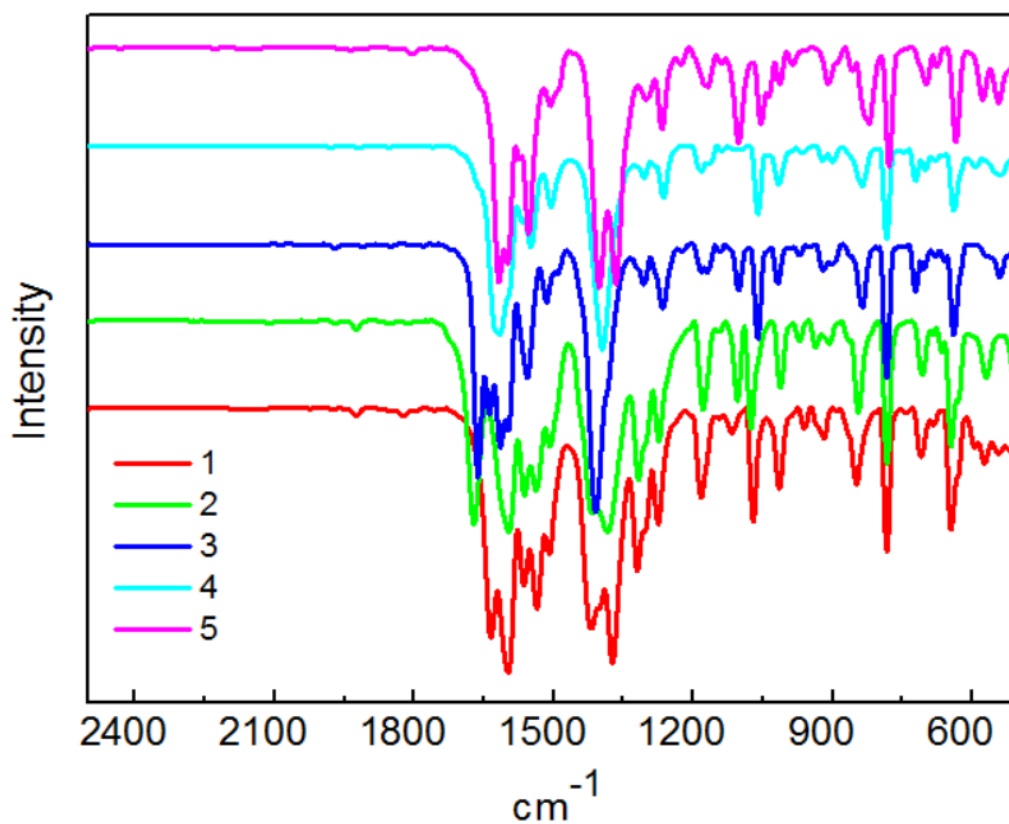[3] B. Bauer, L.D. Carr, H. G. Evertz, A. Feiguin, *J. Stat. Mech*, 2011, P05001.
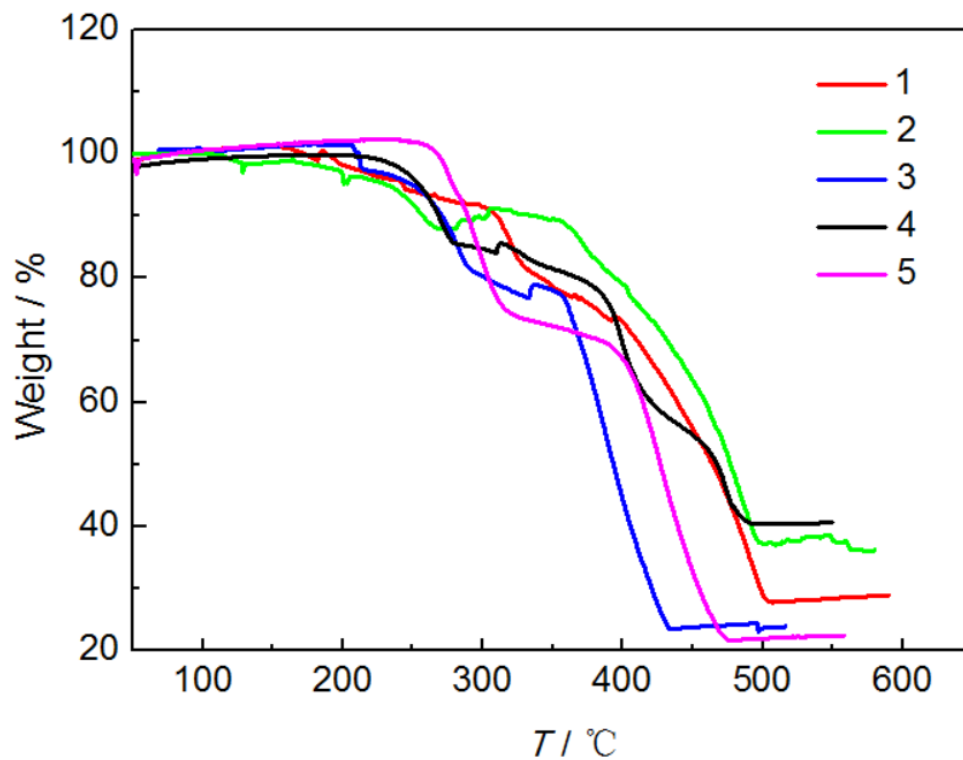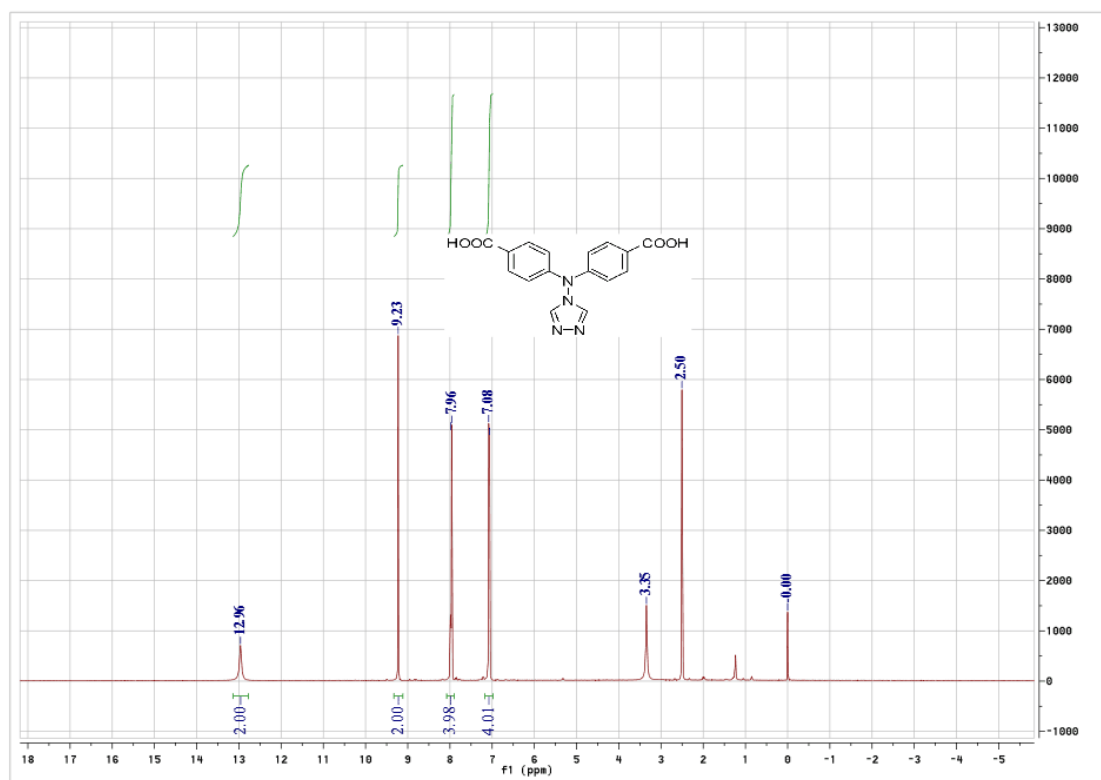
Figure S3. IR spectra of 1-5.

Figure S4. TGA of 1-5



Figure S5. HNMR spectra of H$_2$L