Class II Mesoionic Xanthines as Potential Ten-Qubit Quantum Computer Substrate Registers

*Richard L. Amoroso & Salvatore Giandinoto
*Noetic Advanced Studies Institute, 608 Jean Street, Oakland, CA
noeticj@mindspring.com

Abstract: Class II mesoionic xanthines such as *anhydro*-(8-hydroxyalkyl-5-hydroxy-7-oxothiazolo[3,2-a]pyrimidinium hydroxides) are unique, small atomic weight, stable crystalline organic compounds that can be represented as a combination of ten different resonance structures for each simple xanthine molecule. Each resonance structure contributes a certain percentage to the total resonance of the molecule. This unique resonance represents ten different quantum states of the entire molecule and can thus be exploited as a potential substrate for a ten-qubit register. The number of possible superposition states for such a register in a single molecule is potentially as high as states or (in this case where n = 10) 1,024 complex numbers. In solution the least-unit of this mesoionic crystalline structure is scalable suggesting putative utility for bulk NMR quantum computing. It will be shown that these ten-qubit registers are amenable to standard Deutsch-Jozsa, Shor and Grover algorithms. Additionally, we attempt to formalize I/O techniques for our Class II mesoionic xanthines based on a coherent control RF process of cumulative resonant interaction where by utilizing additional degrees of freedom pertinent to a relativistic basis for the qbit (r-qbit) new HD commutation rules allow decoherence to be ontologically overcome. 2_n

Keywords: Class II Mesoionic Xanthines, Resonance structures, Quantum computing, NMR, algorithms

1. Introduction

Mesoionic purinone analogs, a large and relatively new class of bicyclic heteroaromatic compounds, whose ring systems possess π-electron systems that are isoelectronic with those of the various known purinones, have been synthesized and characterized over the last few decades [1-7]. Class I mesoionic analogs have been classified and defined as being those that are derived from known five-membered mesoionic ring systems. Class II mesoionic analogs are those that are derived from known six-membered mesoionic ring systems. In 1996, Giandinoto, *et.al* [8] had synthesized and characterized a number of novel Class II mesoionic xanthine acyclonucleosides as potential anti-neoplastic and antiviral agents. Class I and Class II mesoioic purinones have been formulated and examined from a quantum chemical standpoint [9-10]. The generalized structural representation of mesoionic xanthine acyclonucleosides is show in Figure 1 below:
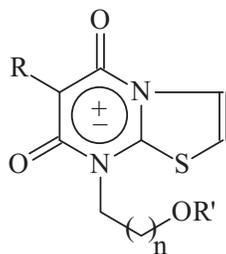
n = 1, 2   R = H, CH$_3$, CH$_3$CH$_2$, C$_6$H$_5$ R' = H, CH$_3$

Figure 1: Generalized structural representation of Class II mesoionic xanthine acyclonucleosides.

In particular, the mesoionic xanthine acyclonucleosides where R' = H are especially useful since this moiety is ideal in giving the molecule a handle for attaching it to metallic, organic, polymeric or semiconductor surfaces/substrates such as GaAs, GaN, CdSe/ZnS. The definition of a mesoionic compound is a compound that cannot be adequately represented by any single covalent or single dipolar resonance structure. These Class II mesoionic xanthines, such as *anhydro*-(8-hydroxyalkyl-5-hydroxy-7-oxothiazolo[3,2a]pyrimidinium hydroxides) cannot be adequately represented by fewer than ten different resonance contributors. Figure 2 illustrates these ten resonance forms and all of their possible quantum inter-conversion states. Each resonance structure shown in Figure 2 corresponds to an individual quantum state of the total molecule and all ten are required to adequately represent the molecule in its totality of superpositional quantum states. In quantum computing, there may be multiple quantum states in superposition. In this particular case where there are ten qubits, the quantum state of superposition would be the following orthonormal basis set:

$$|\psi\rangle = \alpha_i |x_1 x_2 x_3 ... x_n\rangle \text{ for all } i=1\text{-}1,024 \text{ and for all } n=1\text{-}10 \text{ where } x_n \text{ is either 0 or 1.}$$

More succinctly the above may be written: $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |i\rangle$ where $|i\rangle$ is a shorthand notation for an orthonormal basis set of indices $\{i_1, i_2, i_3 ... i_j ... i_n\}$ where $N = 2^n$.

The Greek letters α_i are referred to as the amplitudes of the register and are complex numbers. In a 10-qubit register, there are therefore 2^{10} or 1,024 complex numbers for the total register. Since the probability ($|\Psi|^2$) of a quantum state or set of quantum superpositional entangled states must always be equal to one, the following relationship for the coefficients of the quantum registers must also be true:

$$\sum_{i=1}^{1,024} \alpha_i^2 \equiv |\Psi|^2 = 1$$

For a 3-qubit register, there exists an 8-dimensional complex vector. For a 10-qubit register there exists a 1,024-dimensional complex vector. In order to initialize this vector space (register) for a quantum computer, an algorithm is necessary. In each step of the

algorithm, the vector space is modified by multiplying it with a unitary matrix, which, by definition is a complex matrix.

Resonance Stabilization in Class II Mesoionic Xanthines
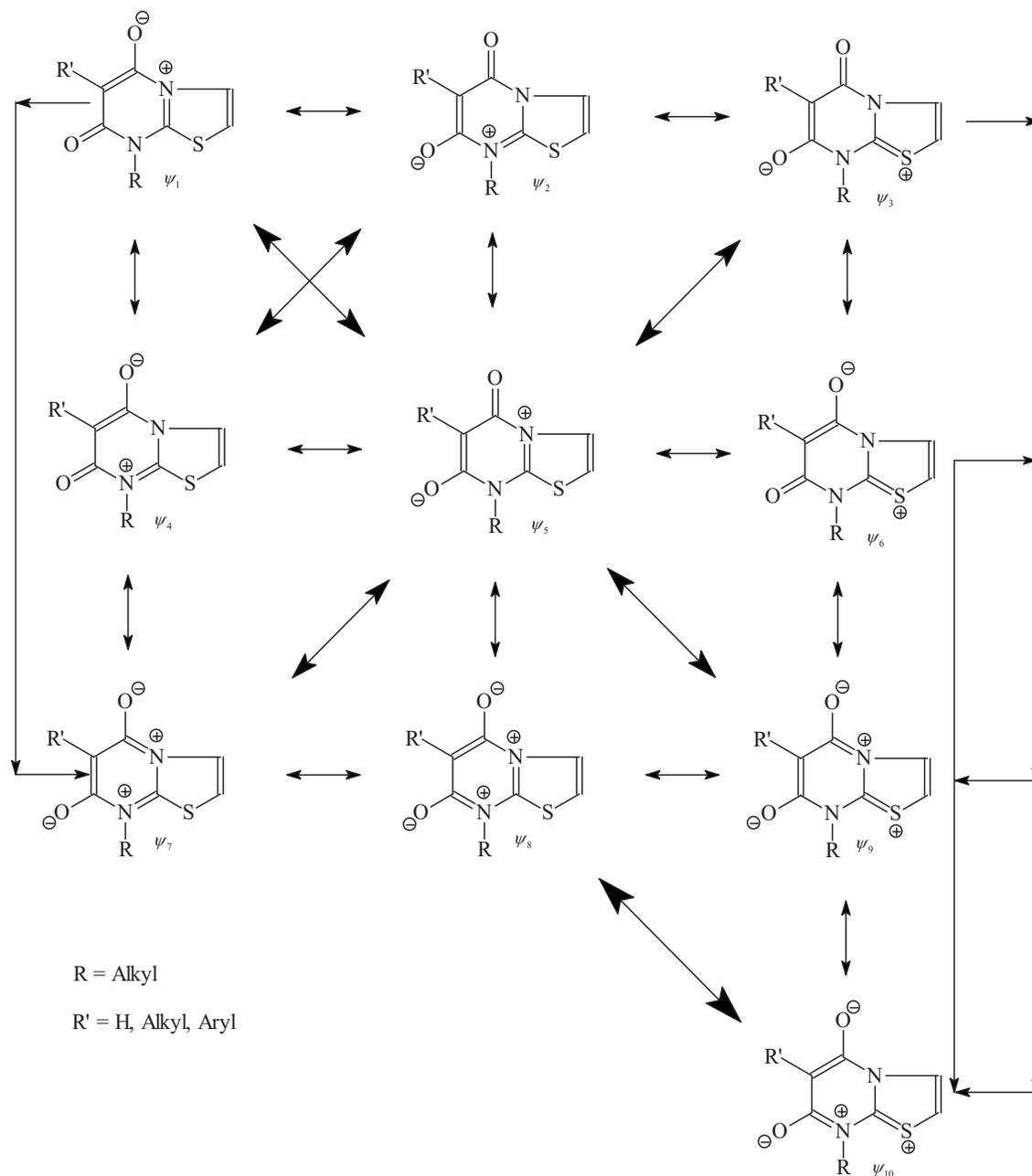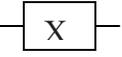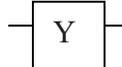

Figure 2: Resonance stabilization in Class II Mesoionic Xanthines

Some of the most important of these unitary transformations or "quantum gates" are the following [11]:

Hadamard Gate: $\boxed{H}$ $\qquad$ $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ $\qquad$ Identity matrix: $I \equiv \sigma_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Pauli –X: $\boxed{X}$ $\qquad$ $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \sigma_x \equiv \sigma_1$ $\qquad$ CNOT Gate: $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

Pauli – Y: $\boxed{Y}$ $\qquad$ $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \sigma_y \equiv \sigma_2$ $\qquad$ Controlled-Z: $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
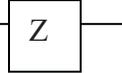
Pauli-Z: $\boxed{Z}$ $\qquad$ $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \sigma_z \equiv \sigma_3$ $\qquad$ Controlled-Phase: $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}$

Phase Gate: $\boxed{S}$ $\qquad$ $\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$

Toffoli Gate: $\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$ $\qquad$ $\pi/8$ Gate: $\boxed{T}$ $\qquad$ $\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$

Since $e^{\pi i} = -1$ and $e^{\pi i/2} = i$, then $e^{\pi i/4} = \sqrt{i}$. Therefore, the $\pi/8$ gate is the square root of the phase gate and the phase gate is consequently the square root of the Pauli-Z gate since $i = \sqrt{-1}$. An operator or matrix is defined as being unitary if the following operation is true: $UU^{-1} = I$. Also, if the complex conjugate transpose of a matrix $U^\dagger$ equals its inverse, U^{-1}, it is considered to be unitary. As an example, the Hermitian conjugate of a matrix A exhibits the following relationship: $A^\dagger = \left(A^T\right)^*$, where A^T is the transpose of the matrix A. Suppose we take the following 3x3 matrix A (where some or all of its elements are complex numbers) and perform the aforementioned operations on it.

$$A^T = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}^T = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}. \quad A^\dagger = \left(A^T\right)^* = \begin{pmatrix} a^*_{11} & a^*_{21} & a^*_{31} \\ a^*_{12} & a^*_{22} & a^*_{32} \\ a^*_{13} & a^*_{23} & a^*_{33} \end{pmatrix}.$$

The matrix $A^\dagger$ is said to be self-adjoint or Hermitian conjugate. Each element of $A^\dagger$ is the complex conjugate of the transpose of A. As another example, let's take the Pauli-Y gate and compute its Hermitian conjugate:

$$\sigma^\dagger_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \sigma_y. \text{ Likewise, for the phase gate } S^\dagger \equiv \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}.$$

Notice that the Hermitian conjugate of the Pauli-Y gate is itself. However, the Hermitian conjugate of the Phase gate S is not equal to itself. Both of these gates are of course unitary since the transpose of their complex conjugates are equal to their inverses.

2. Tensor Products and associated operators.

A tensor product is an operation of putting vector spaces together to form larger vector spaces. This type of construction is absolutely essential to the understanding of the quantum mechanics of multiparticle systems. Let V and W be Hilbert vector spaces of dimension m and n respectively. Then $V \otimes W$ (read 'V tensor W') is a mn-dimensional vector Hilbert space [12]. The elements of $V \otimes W$ are linear combinations of tensor products $|v\rangle \otimes |w\rangle$ of elements $|v\rangle$ of V and $|w\rangle$ of W. Additionally, if $|i\rangle$ and $|j\rangle$ are orthonormal bases for the spaces V and W, then $|i\rangle \otimes |j\rangle$ is a basis for $V \otimes W$. The common abbreviated notations for this type of operation are $|v\rangle|w\rangle, |v, w\rangle \, or \, |vw\rangle$ for the tensor product $|v\rangle \otimes |w\rangle$. Now suppose we introduce the operators A and B that are linear operators on V and W respectively. We can now mathematically show that the following is true: $(A \otimes B)(|v\rangle \otimes |w\rangle) = A|v\rangle \otimes B|w\rangle$. Subsequently, it may also be shown that

$(A \otimes B) \left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle \right) \equiv \sum_i a_i A |v_i\rangle \otimes B |w_i\rangle$. The natural inner product of the spaces

V and W on $V \otimes W$ may now be succinctly defined in terms of the following equation:

$\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle, \sum_j b_j |v_j'\rangle \otimes |w_j'\rangle \right) \equiv \sum_{ij} a_i^* b_j \langle v_i | v_j' \rangle \langle w_i | w_j' \rangle$. This well defined inner

product can be shown in a more concrete manner and a less abstract manner as a matrix or *Kronecker product* whereby A is an m by n matrix and B is a p by q matrix as shown below:

$$A \otimes B \equiv \begin{pmatrix} A_{11}B & \cdots & A_{1n}B \\ \vdots & \ddots & \vdots \\ A_{m1}B & \cdots & A_{mn}B \end{pmatrix}.$$ In this form, terms like $A_{11}B$ refer to p by q sub-matrices

whose entries are proportional to B with the proportionality constant A_{mn}. As an example, the tensor product of the Pauli matrices X and Y is illustrated below:

$$X \otimes Y = \begin{pmatrix} 0Y & 1Y \\ 1Y & 0Y \end{pmatrix} = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}.$$ A close look at the 4X4 matrix shows that the

product of the Pauli matrices X and Y is a compilation of two Pauli-Y matrices that are diagonalized from the upper right of the matrix to the lower left of the matrix with zeros everywhere else. A useful notation for a vector space that is tensored to itself is $|\psi\rangle^{\otimes k}$

where $|\psi\rangle$ is tensored with itself k times. For example, $|\psi\rangle^{\otimes 2} = |\psi\rangle \otimes |\psi\rangle$. Additionally,

the Hadamard transform on n qubits, $H^{\otimes n}$, may be expressed as:

$$H^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x,y} (-1)^{x \cdot y} |x\rangle \langle y|.$$

3. Commutation relations for the Pauli matrices

Two operators are said to *commute* with each other *if and only if* the *commutator* between the two operators is equal to zero. For example the commutator of the Pauli-X and Pauli-Y matrices is shown as follows [13]:

$$[X,Y] \equiv XY - YX = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2iZ$$

Clearly, the Pauli-X and Y matrices are non-commutative as is demonstrated above. If the two operators A and B commute, $[A,B] = 0$ and are said to be *simultaneously diagonalizable*. This occurs *if and only if* there exists an orthonormal basis set (*i.e.,* $|i\rangle$)

that is some common orthonormal set of eigenvectors such that both A and B are diagonal with respect to that basis set. This would be the case if $A = \sum_i a_i |i\rangle\langle i|, B = \sum_i b_i |i\rangle\langle i|$. On the other hand, two operators are said to *anti-commute* if the following operation is true: $\{A, B\} \equiv AB + BA = 0$. A is said to *anti-commute* with B if $\{A, B\} = 0$. The commutation relations for the Pauli matrices are: $[X, Y] = 2iZ$, $[Y, Z] = 2iX$ and $[Z, X] = 2iY$. An elegant way of writing this is by using the **Levi-Civita anti-symmetric permutation tensor** (actually a pseudo-tensor), ε_{jkl} on the three indices where $\varepsilon_{jkl} = 0$ except where $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$ and $\varepsilon_{321} = \varepsilon_{213} = \varepsilon_{132} = -1$. $[\sigma_j, \sigma_k] = 2i \sum_{l=1}^{3} \varepsilon_{jkl} \sigma_l$.

The quantum mechanical operators for linear momentum are shown below [14]:

$\hat{p}_x = -i\hbar \dfrac{\partial}{\partial x}$; $\hat{p}_y = -i\hbar \dfrac{\partial}{\partial y}$; $\hat{p}_z = -i\hbar \dfrac{\partial}{\partial z}$. The operator corresponding to $\hat{p}_x^2$ is

$\hat{p}_x^2 = \left(-i\hbar \dfrac{\partial}{\partial x}\right)^2 = -\hbar^2 \dfrac{\partial^2}{\partial x^2}$ with similar expressions for $\hat{p}_y^2$ and $\hat{p}_z^2$. The commutation

relation for the positional vector $\vec{x}$ and its component linear momentum operator in its

direction is: $\left[\vec{x}, \hat{p}_x\right] = \left[x, -i\hbar \dfrac{\partial}{\partial x}\right] = \left[i\hbar \dfrac{\partial}{\partial x}, x\right] = i\hbar$. Likewise, the commutators for the

positional vectors $\vec{y}$ and $\vec{z}$ and their corresponding component linear momentum

operators ($\hat{p}$ in the same direction) are also equal to $i\hbar$. However, the commutators of the positional vectors in different directions from that of the momentum operators are, of

course, equal to zero (*i.e.*, $\left[\vec{x}, \hat{p}_y\right] = 0$, $\left[\vec{x}, \hat{p}_z\right] = 0$, $\left[\vec{y}, \hat{p}_z\right] = 0$, etc.) and are thus

commutative or said to commute with one another.

The classical mechanical **angular-momentum L** of a particle is described in the following manner: **r** = **i**x + **j**y + **k**z where **r** is the vector from the origin to the instantaneous position of the particle and x, y, and z are the instantaneous coordinates of the particle. Therefore, the particle's **angular-momentum L** with respect to the coordinate origin is $L \equiv r \times p$, where **L** is designated as the following determinant.

$$L = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}.$$ Therefore we have the classical mechanical component **angular-**

momentum vectors: $L_x = yp_z - zp_y$, $L_y = zp_x - xp_z$ and $L_z = xp_y - yp_x$. The **angular-momentum** vector **L** is perpendicular to the plane defined by the particle's position vector **r** and its velocity vector **v** (*i.e.*, **p** = m**v**). However, in the quantum mechanical realm there are two types of angular-momentum: **Orbital angular-momentum** which results from the motion of a particle through space, and is an analog of the classical-mechanical quantity **L** and **spin angular-momentum** which is an intrinsic property of microscopic particles and which therefore has no classical-mechanical analog. The

quantum-mechanical operators for the components of **Orbital angular-momentum** are designated as follows: $\hat{L}_x = -i\hbar\left(y\dfrac{\partial}{\partial z} - z\dfrac{\partial}{\partial y}\right)$, $\hat{L}_y = -i\hbar\left(z\dfrac{\partial}{\partial x} - x\dfrac{\partial}{\partial z}\right)$,

$\hat{L}_z = -i\hbar\left(x\dfrac{\partial}{\partial y} - y\dfrac{\partial}{\partial x}\right)$. Also, $\hat{L}^2 = \left|\hat{L}^2\right| = \hat{L}\bullet\hat{L} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. It may now be shown that the following commutation relations between the *x, y and z* components of the **orbital angular-momentum** operators are as follows: $\left[\hat{L}_x,\hat{L}_y\right] = i\hbar\,\hat{L}_z$ and by performing two successive cyclic permutations on the coordinate indices we naturally obtain

$\left[\hat{L}_y,\hat{L}_z\right] = i\hbar\,\hat{L}_x$ and $\left[\hat{L}_z,\hat{L}_x\right] = i\hbar\,\hat{L}_y$. The components of orbital angular-momentum therefore are non-commutative. Alternatively, however, it may be demonstrated that the total orbital angular-momentum $\hat{L}^2$, commutes with each of its components as is shown below:

$$\left[\hat{L}^2,\hat{L}_x\right] = \left[\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2,\hat{L}_x\right]$$

$$= \left[\hat{L}_x^2,\hat{L}_x\right] + \left[\hat{L}_y^2,\hat{L}_x\right] + \left[\hat{L}_z^2,\hat{L}_x\right]$$

$$= \left[\hat{L}_y^2,\hat{L}_x\right] + \left[\hat{L}_z^2,\hat{L}_x\right]$$

$$= \left[\hat{L}_y,\hat{L}_x\right]\hat{L}_y + \hat{L}_y\left[\hat{L}_y,\hat{L}_x\right] + \left[\hat{L}_z,\hat{L}_x\right]\hat{L}_z + \hat{L}_z\left[\hat{L}_z,\hat{L}_x\right]$$

$$= -i\hbar\,\hat{L}_z\,\hat{L}_y - i\hbar\,\hat{L}_y\,\hat{L}_z + i\hbar\,\hat{L}_y\,\hat{L}_z + i\hbar\,\hat{L}_z\,\hat{L}_y$$

$$\left[\hat{L}^2,\hat{L}_x\right] = 0$$

Likewise, of course, the total angular-momentum operator also commutes with its *y* and *z* components L_y and L_z and therefore the commutation relations between $\hat{L}^2$ and these components are also zero. Analogous to the aforementioned orbital angular-momentum operators we also have the **spin angular-momentum** operators $\hat{S}^2,\hat{S}_x,\hat{S}_y,\hat{S}_z$ which are both linear and Hermitian [15]. $\hat{S}^2$ is the operator for the square of the magnitude of the total spin angular-momentum of a particle. As before with the orbital angular-momentum, we have $\hat{S}^2 = \hat{S}_x + \hat{S}_y + \hat{S}_z$. Also, as before, we have the following similar commutation relations for the spin angular-momentum operators: $\left[\hat{S}_x,\hat{S}_y\right] = i\hbar\,\hat{S}_z$,

$$\left[\hat{S}_y, \hat{S}_z\right] = i\hbar\,\hat{S}_x \text{ and } \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\,\hat{S}_y.$$ Additionally, the **total spin angular-momentum**

operators have the following commutation relations: $\left[\hat{S}^2, \hat{S}_x\right] = \left[\hat{S}^2, \hat{S}_y\right] = \left[\hat{S}^2, \hat{S}_z\right] = 0$.

4. Quantum Superposition and quantum probabilities of the 10-qubit mesoionic registers

Quantum mechanically speaking, the ground and various excited state(s) of the mesoionic xanthines represented in Figure 2 have the ability to exist in a total superposition of ten different quantum states simultaneously. It is this feature of these mesoionic xanthines that we attempt to exploit in terms of their utilization as potential substrates for 10-qubit quantum computer registers. Each resonance structure depicted in Fig. 2 is a distinct quantum state and can therefore be represented by a distinct wavefunction ψ_i. We therefore have ten different wavefunctions that can exist in a quantum superpositional and quantum entangled state that may be represented by the following linear combination of wavefunctions: $\Psi = \psi_1 + \psi_2 + \psi_3 + ... + \psi_{10}$. The state Ψ is the maximally entangled quantum state of the molecule and is therefore the lowest energy state or **ground state** of the molecule.

Each resonance structure depicted in Fig. 2 has a certain probability associated with that particular state. We determine these probabilities by utilizing a fundamental rule in quantum chemistry. This rule basically states the following: ***The number of possible resonance inter-conversion states a particular resonance structure possesses is directly proportional to the probability of that quantum state.*** As a few examples, using Fig. 2, let us first take a look at the most probable resonance structure which is designated as ψ_5. Resonance structure or quantum state ψ_5 has a total of **8** possible resonance inter-conversions. These eight inter-conversions of quantum state ψ_5 are with the following quantum states: $\psi_1, \psi_2, \psi_3, \psi_4, \psi_6, \psi_7, \psi_8, \psi_9$. This is therefore the most probable quantum state of the molecule. As another example, let us count the number of possible inter-conversion states for ψ_1. This state inter-converts with $\psi_2, \psi_4, \psi_5, \psi_7$ or a total of four quantum states. The list of possible inter-conversion states possible for each of the ten quantum states is listed below:

$$\psi_1 = 4 \qquad \psi_6 = 4$$
$$\psi_2 = 4 \qquad \psi_7 = 4$$
$$\psi_3 = 5 \qquad \psi_8 = 4$$
$$\psi_4 = 4 \qquad \psi_9 = 5$$
$$\psi_5 = 8 \qquad \psi_{10} = 4$$

The total number of quantum resonance inter-conversions is therefore equal to 46. It is now a rather trivial procedure to calculate the actual probabilities in terms of coefficients of the individual quantum states. We simply take the above numbers for each state and

divide them by the total number of inter-conversion states. The following probabilities are thus obtained:

$$\alpha_1^2 = \frac{2}{23} \qquad \alpha_6^2 = \frac{2}{23}$$

$$\alpha_2^2 = \frac{2}{23} \qquad \alpha_7^2 = \frac{2}{23}$$

$$\alpha_3^2 = \frac{5}{46} \qquad \alpha_8^2 = \frac{2}{23}$$

$$\alpha_4^2 = \frac{2}{23} \qquad \alpha_9^2 = \frac{5}{46}$$

$$\alpha_5^2 = \frac{4}{23} \qquad \alpha_{10}^2 = \frac{2}{23}$$

We may now re-write the total wavefunction Ψ in the following manner:

$$\Psi = \frac{2}{23}\psi_1 + \frac{2}{23}\psi_2 + \frac{5}{46}\psi_3 + \frac{2}{23}\psi_4 + \frac{4}{23}\psi_5 + \frac{2}{23}\psi_6 + \frac{2}{23}\psi_7 + \frac{2}{23}\psi_8 + \frac{5}{46}\psi_9 + \frac{2}{23}\psi_{10},$$

where all of the coefficients of the individual wavefunctions add up to equal one. We may also express the above wavefunction in our more familiar quantum computer form as:

$$|\Psi\rangle = \sum_{i=1}^{N} \sqrt{\tfrac{2}{23}}|i\rangle + \sqrt{\tfrac{2}{23}}|i\rangle + \sqrt{\tfrac{5}{46}}|i\rangle + \sqrt{\tfrac{2}{23}}|i\rangle + \tfrac{2}{\sqrt{23}}|i\rangle + \sqrt{\tfrac{2}{23}}|i\rangle + \sqrt{\tfrac{2}{23}}|i\rangle + $$

$$\sqrt{\tfrac{2}{23}}|i\rangle + \sqrt{\tfrac{5}{46}}|i\rangle + \sqrt{\tfrac{2}{23}}|i\rangle$$

or more succinctly as: $|\Psi\rangle = \sum_{i=1}^{N} 7\sqrt{\tfrac{2}{23}}|i\rangle + \tfrac{2}{\sqrt{23}}|i\rangle + 2\sqrt{\tfrac{5}{46}}|i\rangle$, where

$|i\rangle = \{i_1, i_2, i_3 ... i_j ... i_n\}$ and $n = 10$; $N = 1,024$.

5. Projectors and Projection Operators

Let us examine the role of projectors and projection operators. A projection matrix P is an n x n square matrix that gives a vector space projection from R^n to a subspace W. The columns of P are the projections of the standard basis vectors and W is the image of P. Therefore, a square matrix P is a projection matrix *if and only if* $P^2 = P$. A projection matrix P is orthogonal *if and only if* $P = P^{\dagger}$.

Suppose W is a k-dimensional subspace of the d-dimensional vector space V. Using the **Gram-Schmidt** procedure, it is possible to construct an orthonormal basis $|1\rangle, ..., |d\rangle$ for V such that $|1\rangle, ..., |k\rangle$ is an orthonormal basis for W. We may represent this definition mathematically by stating that the projector P is the projector onto the subspace W using

the following equation [16]: $P \equiv \sum_{i=1}^{k} |i\rangle\langle i|$. It can easily be shown that this definition is independent of the orthonormal basis $|1\rangle,...,|k\rangle$ used for W. It can further be shown that $|v\rangle\langle v|$ is Hermitian for any vector $|v\rangle$ and so P is Hermitian, $P^\dagger = P$. We may now refer to P as the vector space onto which P is a projector. The *orthogonal complement* of P is the operator $Q \equiv I - P$. The operator Q is therefore a projector onto the vector space spanned by $|k+1\rangle,...|d\rangle$ which we also refer to as the *orthogonal complement* of P, and may denote by Q.

6. The Density Operator, Measurement Operator and Ensembles of Quantum States

Thus far, we have formulated our quantum mechanics using the concept or language of state vectors. An alternative formalism that is mathematically equivalent to the state vector approach is that of the density operator or density matrix. The density operator approach provides a much more convenient way for representing some commonly encountered scenarios within the framework of quantum mechanics. Suppose the quantum system is in one of a number of quantum states $|\psi_i\rangle$, where i is an index with respective probabilities p_i. We shall then call $\{p_i, |\psi_i\rangle\}$ an *ensemble of pure states*. The density operator for the system is defined by the following equation [17]: $\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|$. As stated previously, the density operator is also known as the density matrix. The two terms may be used interchangeably. All of the postulates of quantum mechanics can be reformulated or expressed in terms of the density operator language. Both the density operator language and the state vector language give the exact same results, however the use of one over the other may make it easier to approach problems from one point of view rather than the other. Suppose that the evolution of a closed quantum system is described by the unitary operator U. If the system was initially in the state $|\psi_i\rangle$, with probability p_i then after the evolution has occurred the system will be in the state $U|\psi_i\rangle$ with probability p_i. This is shown mathematically below:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger.$$

The measurement operators M_m may also be described in terms of the density operator language. If the initial state of a quantum system is $|\psi_i\rangle$ then the probability of getting a result m is: $p(m|i) = \langle\psi_i|M_m^\dagger M_m|\psi_i\rangle = \text{tr}\left(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|\right)$, where we have used the known relationship, $\text{tr}\left(A|\psi\rangle\langle\psi|\right) = \sum_i\langle i|A|\psi\rangle\langle\psi|i\rangle = \langle\psi|A|\psi\rangle$ where the end result is that the operator is sandwiched between the two wavefunctions or quantum states. The notation whereby the operator, usually the Hamiltonian, is sandwiched between the two states is very common in quantum mechanics. Therefore, the probability of obtaining result m is: $p(m) = \sum_i p(m|i)p_i = \sum_i p_i\text{tr}\left(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|\right) = \text{tr}\left(M_m^\dagger M_m\rho\right)$.

Now suppose we wish to determine the density operator of the system after making the measurement m. If the initial state was $|\psi_i\rangle$ then the state after the measurement m is:

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{\sqrt{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}}.$$ After the measurement that yields the result m we have an

ensemble of states $|\psi_i^m\rangle$ with respective probabilities $p(i|m)$ with the corresponding

density operator $\rho_m = \sum_i p(i|m)|\psi_i^m\rangle\langle\psi_i^m| = \sum_i p(i|m)\frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle}$. Using the

following definitions for probability theory, $p(i|m) = \frac{p(m,i)}{p(m)} = \frac{p(m,i)p_i}{p(m)}$ and with the

appropriate substitutions, we may further show that the following is true:

$$\rho_m = \sum_i p_i \frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\text{tr}\left(M_m^\dagger M_m\rho\right)} = \frac{M_m\rho M_m^\dagger}{\text{tr}\left(M_m^\dagger M_m\rho\right)}.$$ We have thus proven that the basic

postulates of quantum mechanics related to the unitary evolution and measurement can be viewed in terms of the density operator formalism. Furthermore, a quantum system whose state $|\psi\rangle$ is known exactly is said to be in a *pure state* (i.e., $\rho = |\psi\rangle\langle\psi|$). If the state function is not known exactly, then the density operator ρ is said to be in a *mixed state* which is simply a *mixture* of the different pure states in the ensemble for ρ. It may also be easily shown that for a pure state $\text{tr}(\rho^2) = 1$ and for a mixed state $\text{tr}(\rho^2) < 1$. Now suppose we have a quantum system in the state ρ_i with a probability p_i. The system may therefore be described by the density matrix $\sum_i p_i\rho_i$. This can be proven by assuming that ρ_i arises from some ensemble of $\{p_{ij}, |\psi_{ij}\rangle\}$ pure states (where i is fixed) so that the probability for being in the state $|\psi_{ij}\rangle$ is thus p_ip_{ij}. The density matrix for this system is thus: $\rho = \sum_{ij} p_ip_{ij}|\psi_{ij}\rangle\langle\psi_{ij}| = \sum_i p_i\rho_i$, where the we have used the definition $\rho_i = \sum_j p_{ij}|\psi_{ij}\rangle\langle\psi_{ij}|$. We conclude that ρ is therefore a *mixture* of the states ρ_i with probabilities p_i.

7. Time evolution of the state-function of a closed quantum system

The time evolution of a state function is given by the well known *Schrödinger equation,*

$$i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle$$ where H is the *Hamiltonian* of the closed system [18]. Due to the fact

the Hamiltonian is a Hermitian operator, it has a spectral decomposition:

$$H = \sum_E E|E\rangle\langle E|$$ which includes the eigenvalues E and their corresponding eigenvectors

$|E\rangle$. The states $|E\rangle$ are referred to as the *energy eigenstates* or as *stationary states*, and E

is the energy of of the state $|E\rangle$. The lowest energy is known as the *ground state energy* and the corresponding energy eigenstate is known as the *ground state.* The energy eingenstates $|E\rangle$ are known as stationary states since their only change in time is to acquire an overall numerical factor, $|E\rangle \rightarrow e^{(-iEt/\hbar)}|E\rangle$. A simple example would be to consider a single qubit having the following Hamiltonian, $H = \hbar\omega X$, where $\omega = 2\pi f$ and f is the frequency of the particle or photon. The energy eigenstates of this Hamiltonian are $\dfrac{|0\rangle \pm |1\rangle}{\sqrt{2}}$ with corresponding energies $\hbar\omega$ and $-\hbar\omega$. The ground state is therefore $-hf$ and the ground state energy is $-\hbar\omega$ or $-hf$. The solution to the Schrödinger equation utilizing the unitary operator U is shown below:

$$|\psi(t_2)\rangle = e^{\left[\frac{-iH(t_2-t_1)}{\hbar}\right]}|\psi(t_1)\rangle = U(t_1,t_2)|\psi(t_1)\rangle, \text{ where } U(t_1,t_2) \equiv e^{\left[\frac{-iH(t_2-t_1)}{\hbar}\right]}.$$

Furthermore, it may be shown that any unitary operator U can be expressed in the compact form $U = e^{iK}$ for any Hermitian operator K.

8. Quantum Simulations of Hamiltonians

Quantum simulations have largely concentrated on simulating Hamiltonians that are sums of local interactions. However, this is not a fundamental requirement! Efficient quantum simulations are possible even for Hamiltonians which act non-trivially on all parts of a large quantum system. Suppose we have the Hamiltonian: $H = Z_1 \otimes Z_2 \otimes ... \otimes Z_n$ which acts on an *n*-qubit system. We may apply a Hermitian phase shift $e^{-i\Delta t}$ to the system if the parity of the *n*-qubits in the computational basis set is even. If odd, the phase shift is $e^{i\Delta t}$. We may therefore efficiently simulate any Hamiltonian of the form: $H = \bigotimes\limits_{k=1}^{n} \sigma_{c(k)}^{k}$,

where $\sigma_{c(k)}^{k}$ is a Pauli matrix or the identity acting on the kth-qubit, with $c(k) \in \{0,1,2,3\}$ designating one of the matrices $\{I, X, Y, Z\}$. There are a couple of useful algebraic facts regarding the various quantum gates such as the Hadamard gate (H) and the various Pauli, phase and π/8-gates. The Hadamard gate $H = (X + Z)/\sqrt{2}$ and the phase-gate $S = T^2$. The T-gate or π/8-gate is called such since it contains $e^{\pm i\pi/8}$ appearing on its diagonals [19]: $T = e^{i\pi/8}\begin{pmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{pmatrix}$. For a single qubit-vector state $|\psi\rangle = a|0\rangle + b|1\rangle$

parameterized by two complex numbers satisfying the relationship $|a|^2 + |b|^2 = 1$, the state may be visualized as a point (θ, φ) on the unit sphere where $a = \cos\left(\dfrac{\theta}{2}\right)$ and $b = e^{i\varphi}\sin\left(\dfrac{\theta}{2}\right)$. This is known as the Bloch sphere representation and the vector $(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$ is known as the Bloch vector. The value for a can be taken

as a real number since the overall phase of the state is unobservable. Additionally, upon exponentiation, the Pauli matrices give rise to a very useful class of unitary matrices known as *rotation operators* about the *x, y* and *z* axes, defined by the equations below:

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}X = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Y = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Z = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

9. Initialization of Mesoionic Xanthine registers

The mesoionic xanthine molecule, as depicted in Fig. 2, represents a molecule that is in a quantum superposition of at least ten distinct and unique quantum states. An efficient scheme for initializing quantum registers with an arbitrary superposed state, without the introduction of additional qubits (Ventura & Martinez 1999 [20]) has been developed by Long & Sun [21]. This scheme begins with the state $|0...0\rangle$ and is then transformed to a general superposed state of the following form: $|\psi\rangle = \sum_{i=0}^{N-1} a_i |i\rangle$. In this particular case, $N = 1,024$ and $|i\rangle$ is the shorthand notation for the basis set $\{i_1, i_2, i_3...i_j...i_n\}$ where $n = \log_2 N$ and where i_j denotes the two possible states (0 or 1) of the jth-qubit. The following diagram will illustrate this concept more easily:

$$i = \begin{cases} 0 \rightarrow \{000...000\} \\ 1 \rightarrow \{000...001\} \\ 2 \rightarrow \{000...010\} \\ 3 \rightarrow \{000...100\} \\ . \\ . \\ . \\ N-1 \rightarrow \{111,...111\} \end{cases}$$

The above diagram therefore illustrates that $|\psi\rangle$ is a general quantum superposition of N basis states and each basis state is a product state of n qubits. The initialization scheme involves only two types of unitary transformations or gate operations. The first gate

operation is a single bit rotation U_θ, $U_\theta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. This rotation differs

from an ordinary rotation because it is an ordinary rotation only for the $|0\rangle$ bit but interjects a minus sign for the $|1\rangle$ bit. The operation thus converts a qubit in the state $|0\rangle$ to a superposition of the two state $(\cos\theta, \sin\theta)$ and a qubit in the $|1\rangle$ state to the superposition of the two state $(\sin\theta, -\cos\theta)$. When $\theta = 0$, the state $|0\rangle$ remains unchanged but converts the sign of state $|1\rangle$ (i.e., Pauli-Z gate). When $\theta = \dfrac{\pi}{4}$, U_θ is simply reduced to the Hadamard-Walsh transformation. When $\theta = \dfrac{\pi}{2}$ ($90°$ rotation), it acts as the NOT operation (Pauli-X, σ_x) by changing $|0\rangle$ to $|1\rangle$ and $|1\rangle$ to $|0\rangle$.

The second type of gate operation is known as the controlled^k-operation. This operation is constructed from a string of k controlling qubits as shown below:
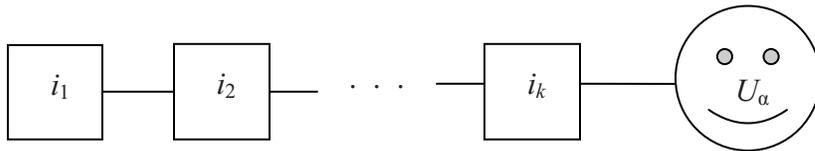
The squares represent the controlling qubits $\{i_1, i_2, ...i_k\}$ and the circle is a unitary operation on the target qubit representing an angle of rotation. The uniqueness and power of this operation is that it is a conditional one that is activated only when the controlling qubits hold the respective values indicated in the squares. Controlled^k-operations may be constructed using $O(k^2)$ standard 1- and 2-bit gate operations [22]. In order to more easily see how these operations are performed we may take a look at the simple example of a two qubit system.

$$|00\rangle \rightarrow \sqrt{|a_{00}|^2 + |a_{01}|^2}\, |00\rangle + \sqrt{|a_{10}|^2 + |a_{11}|^2}\, |10\rangle \qquad \text{Operation 1.) Single bit rotation } \alpha_1,$$

$$\rightarrow |0\rangle \big[a_{00} |0\rangle + a_{01} |1\rangle \big] + |1\rangle \big[a_{10} |0\rangle + a_{11} |1\rangle \big] \qquad \text{Operation 2.) Two controlled}^1\text{-}$$
$$\text{operations } U_{\alpha 2, i} \ (i = 0, 1).$$

$$= a_{00} |00\rangle + a_{01} |01\rangle + a_{10} |10\rangle + a_{11} |11\rangle$$

The single bit rotation α_1 is equal to $\tan^{-1} \sqrt{\dfrac{|a_{10}|^2 + |a_{11}|^2}{|a_{00}|^2 + |a_{01}|^2}}$. We may now represent the operations in matrix form as well:

$$U_{\alpha 2,0} = \begin{bmatrix} \dfrac{a_{00}}{\sqrt{|a_{00}|^2 + |a_{01}|^2}} & \dfrac{a_{01}}{\sqrt{|a_{00}|^2 + |a_{01}|^2}} \\[2em] \dfrac{a_{01}^*}{\sqrt{|a_{00}|^2 + |a_{01}|^2}} & \dfrac{a_{00}^*}{\sqrt{|a_{00}|^2 + |a_{01}|^2}} \end{bmatrix} \qquad U_{\alpha 2,1} = \begin{bmatrix} \dfrac{a_{10}}{\sqrt{|a_{10}|^2 + |a_{11}|^2}} & \dfrac{a_{11}}{\sqrt{|a_{10}|^2 + |a_{11}|^2}} \\[2em] \dfrac{a_{11}^*}{\sqrt{|a_{10}|^2 + |a_{11}|^2}} & \dfrac{a_{10}^*}{\sqrt{|a_{10}|^2 + |a_{11}|^2}} \end{bmatrix}$$

The situation becomes even more interesting when using a larger register such as a 3-qubit register having 8 basis states:

1. Starting from the state $|000\rangle$, a single bit rotation is operated on the 1st-qubit with the angle $\alpha_1 = \tan^{-1}\sqrt{\dfrac{|a_{100}|^2 + |a_{101}|^2 + |a_{110}|^2 + |a_{111}|^2}{|a_{000}|^2 + |a_{001}|^2 + |a_{010}|^2 + |a_{011}|^2}}$ transforming the initialized state $|000\rangle$ to the state $\sqrt{|a_{000}|^2 + |a_{001}|^2 + |a_{010}|^2 + |a_{011}|^2}\,|000\rangle + \sqrt{|a_{100}|^2 + |a_{101}|^2 + |a_{110}|^2 + |a_{111}|^2}\,|100\rangle$.

2. Then, two controlled[1]-rotations with angles

$$\tan^{-1}\sqrt{\dfrac{|a_{010}|^2 + |a_{011}|^2}{|a_{000}|^2 + |a_{001}|^2}} \quad \text{and} \quad \tan^{-1}\sqrt{\dfrac{|a_{110}|^2 + |a_{111}|^2}{|a_{100}|^2 + |a_{101}|^2}}$$ operate on the 2nd-qubit. The resulting

superposed state vector therefore becomes:

$$\sqrt{|a_{000}|^2 + |a_{001}|^2}\,|000\rangle + \sqrt{|a_{010}|^2 + |a_{011}|^2}\,|010\rangle + \sqrt{|a_{100}|^2 + |a_{001}|^2}\,|100\rangle + \sqrt{|a_{110}|^2 + |a_{111}|^2}\,|110\rangle.$$

3. Finally, 4 controlled[2]-unitary transformations operate on the 3rd-qubit to generate the superposed state:

$$a_{000}|000\rangle + a_{001}|001\rangle + a_{010}|010\rangle + a_{100}|100\rangle + a_{011}|011\rangle + a_{101}|101\rangle + a_{110}|110\rangle + a_{111}|111\rangle.$$

These 4 controlled[2]-unitary transformations are:

$$U_{\alpha 3,00} = \begin{bmatrix} \dfrac{a_{000}}{\sqrt{|a_{000}|^2 + |a_{001}|^2}} & \dfrac{a_{001}}{\sqrt{|a_{000}|^2 + |a_{001}|^2}} \\[2em] \dfrac{a_{001}^*}{\sqrt{|a_{000}|^2 + |a_{001}|^2}} & -\dfrac{a_{000}^*}{\sqrt{|a_{000}|^2 + |a_{001}|^2}} \end{bmatrix}$$

$$U_{\alpha 3,01} = \begin{bmatrix} \dfrac{a_{010}}{\sqrt{|a_{010}|^2 + |a_{011}|^2}} & \dfrac{a_{011}}{\sqrt{|a_{010}|^2 + |a_{011}|^2}} \\[2em] \dfrac{a_{011}^*}{\sqrt{|a_{010}|^2 + |a_{011}|^2}} & -\dfrac{a_{010}^*}{\sqrt{|a_{010}|^2 + |a_{011}|^2}} \end{bmatrix}$$

$$U_{\alpha3,10} = \begin{bmatrix} \dfrac{a_{100}}{\sqrt{|a_{100}|^2 + |a_{101}|^2}} & \dfrac{a_{101}}{\sqrt{|a_{100}|^2 + |a_{101}|^2}} \\ \dfrac{a_{101}^*}{\sqrt{|a_{100}|^2 + |a_{101}|^2}} & -\dfrac{a_{100}^*}{\sqrt{|a_{100}|^2 + |a_{101}|^2}} \end{bmatrix}$$

$$U_{\alpha3,11} = \begin{bmatrix} \dfrac{a_{110}}{\sqrt{|a_{110}|^2 + |a_{111}|^2}} & \dfrac{a_{111}}{\sqrt{|a_{110}|^2 + |a_{111}|^2}} \\ \dfrac{a_{111}^*}{\sqrt{|a_{110}|^2 + |a_{111}|^2}} & -\dfrac{a_{110}^*}{\sqrt{|a_{110}|^2 + |a_{111}|^2}} \end{bmatrix}$$

For notation purposes we use an "angle" to label a controlled^k-operation. If the coefficients are all real, it reduces to an ordinary rotation angle. The notations of angles of the controlled^k-rotations, the first subscript designates the target qubit order number and the subscripts following the comma designate the quantum states of the controlling qubits. For example, 3 in $\alpha_{3,11}$ refers to the target qubit and the subscripts (11 in $\alpha_{3,11}$) refer to the controlling qubits. In the initialization, operations for the first $n-1$ qubits are controlled rotations where each rotation depends only on a single real parameter. The rotation angles take on the following general expressions. In the first qubit there is a 1-qubit rotation. The rotation angle is: $\alpha_1 = \tan^{-1}\sqrt{\dfrac{\sum_{i_2 i_3 \dots i_n} |a_{1 i_2 i_3 \dots i_n}|^2}{\sum_{i_2 i_3 \dots i_n} |a_{0 i_2 i_3 \dots i_n}|^2}}$. In the 2$^{\text{nd}}$-qubit, there are two controlled^1-rotations:

$$\alpha_{2,0} = \tan^{-1}\sqrt{\dfrac{\sum_{i_3 i_4 \dots i_n} |a_{01 i_3 i_4 \dots i_n}|^2}{\sum_{i_3 i_4 \dots i_n} |a_{00 i_3 i_4 \dots i_n}|^2}} \quad \text{and} \quad \alpha_{2,1} = \tan^{-1}\sqrt{\dfrac{\sum_{i_3 i_4 \dots i_n} |a_{11 i_3 i_4 \dots i_n}|^2}{\sum_{i_3 i_4 \dots i_n} |a_{10 i_3 i_4 \dots i_n}|^2}}$$. In general, in the jth-qubit, there are 2^{j-1} controlled^{j-1}-rotations, with each of them having j - 1 controlling qubits labeled as $i_1 i_2 \dots i_{j-1}$. The rotation angle in the jth-qubit ($j \neq n$) is given by:

$$\alpha_{j, i_1 i_2 \dots i_{j-1}} = \tan^{-1}\sqrt{\dfrac{\sum_{i_{j+1} \dots i_n} |a_{i_1 i_2 \dots i_{j-1} 1 i_{j+1} \dots i_n}|^2}{\sum_{i_{j+1} \dots i_n} |a_{i_1 i_2 \dots i_{j-1} 0 i_{j+1} \dots i_n}|^2}} .$$

For the last qubit, where $j = n$ we have 2^{n-1} controlled^{n-1} unitary transformations where:

$$U_{\alpha_{n,i_1i_2\ldots i_{n-1}}} = \begin{bmatrix} \dfrac{A_0}{\sqrt{|A_0|^2+|A_1|^2}} & \dfrac{A_1}{\sqrt{|A_0|^2+|A_1|^2}} \\ \dfrac{A_1^*}{\sqrt{|A_0|^2+|A_1|^2}} & -\dfrac{A_0^*}{\sqrt{|A_0|^2+|A_1|^2}} \end{bmatrix}$$ where $A_0 = a_{i_1i_2\ldots i_{n-1}0}$ and $A_1 = a_{i_1i_2\ldots i_{n-1}1}$.

If A_0 and A_1 are real, the operation is simply a rotation and the angle is given by:

$$\alpha_{n,i_1i_2\ldots i_{n-1}} = \tan^{-1}\left(\frac{A_1}{A_0}\right).$$

We are now ready to initialize quantum superposition registers of three different types starting from the state $|0\ldots0\rangle$:

1. The evenly distributed state $|\psi\rangle = \sum_i |i\rangle$ is the most common state in quantum computing. The Hadamard-Walsh gate operation on each qubit generates this form of superposition from the state $|0\ldots0\rangle$. In this particular case, all of the rotation angles are $\pi/4$. In each qubit, the controlling qubits use up all possible combinations and therefore the 2^{j-1} controlled Hadamard-Wash gate operations are reduced to a single Hadamard-Walsh transformation in the jth-qubit.

2. The Greenberger-Horne-Zeilinger or GHZ state is the maximally entangled state with the superposition $\frac{1}{\sqrt{2}}(|0\ldots0\rangle \pm |1\ldots1\rangle)$. Suppose we would like to transform the state $|0000\rangle$ to the state $\frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$. The circuit below shows this diagrammatically:
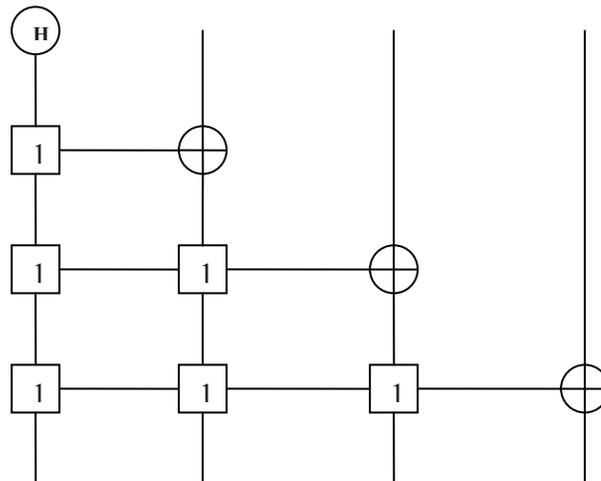
Quantum Circuit for the GHZ state
Figure 3

The rotation in the 1st-qubit is the Hadamard-Walsh transformation. There are two controlled operations $\alpha_{2,0} = 0$ in the 2nd-qubit that are equal to the identity operation and so does nothing to the qubit. However $\alpha_{2,1} = \dfrac{\pi}{2}$ corresponds to the CNOT operation, so effectively, there is only one controlled-NOT gate in the 2nd-qubit. There are four gate operations in the 3rd-qubit. $\alpha_{3,11} = \dfrac{\pi}{2}$ is the $|11\rangle$-CNOT gate and $\alpha_{3,00}$ is the identity operation. $\alpha_{3,01}$ and $\alpha_{3,10}$ are undetermined angles equal to $\dfrac{0}{0}$. Upon closer examination, however, these angles are equal to 0 and are therefore equal to the identity operation. Therefore, the only gate operation in the 3rd-qubit is the $|11\rangle$-CNOT operation. Similarly, there is only the $|111\rangle$-CNOT operation in the 4th-qubit. Should the circuit contain more than four qubits, the same analysis applies until the last qubit. For the last qubit, the rotation is either $\dfrac{\pi}{2}$ for the state $\dfrac{1}{\sqrt{2}}\left(|0...0\rangle+|1...1\rangle\right)$ or $-\dfrac{\pi}{2}$ for the state $\dfrac{1}{\sqrt{2}}\left(|0...0\rangle-|1...1\rangle\right)$.

3. In the Grover search algorithm [23], the state vector is built up in a two-dimensional space spanned by the so-called "marked" state $|\tau\rangle$ and the "rest" state $|c\rangle = \sum_{i \neq \tau}|i\rangle$. At any step in the search, the state vector has the form $|\psi\rangle = \sin\theta|\tau\rangle + \cos\theta|c\rangle$. In order to initialize such a superposed state, we let $|\tau\rangle = |i_1 i_2 ... i_n\rangle$ be the marked state. We may now construct the state $|\psi\rangle$ from $|0...0\rangle$. The amplitudes a_i of the basis states $|\psi\rangle = \sum_{i=0}^{N-1} a_i |i\rangle$ are $a_\tau = \sin\theta$ and $a_i = \cos\theta/\sqrt{N-1}$ for $i \neq \tau$. According to the following equation,

$$\alpha_1 = \tan^{-1}\sqrt{\frac{\sum_{i_2 i_3 ... i_n}\left|a_{1 i_2 i_3 ... i_n}\right|^2}{\sum_{i_2 i_3 ... i_n}\left|a_{0 i_2 i_3 ... i_n}\right|^2}}\,,$$ the rotation angle in the 1st-qubit is:

$$\alpha_1 = \begin{cases} \tan^{-1}\Omega_1, & \text{if } i_1 = 1 \\ \tan^{-1}\dfrac{1}{\Omega_1}, & \text{if } i_1 = 0 \end{cases} \quad \text{where } \Omega_1 = \sqrt{\frac{(N-2)\cos^2\theta + 2(N-1)\sin^2\theta}{N\cos^2\theta}}\,. \quad \text{In the } k^{\text{th}}\text{-qubit,}$$

the angle for the $|i_1, i_2 ... i_{k-1}\rangle$-controlled rotation is therefore:

$$\alpha_{k,i_1,i_2\ldots i_{k-1}} = \begin{cases} \tan^{-1}\Omega_k, & \text{if } i_k = 1 \\ \tan^{-1}\dfrac{1}{\Omega_k}, & \text{if } i_k = 0 \end{cases} \quad \text{where } \Omega_1 = \sqrt{\dfrac{\left(N - 2^k\right)\cos^2\theta + 2^k\left(N-1\right)\sin^2\theta}{N\cos^2\theta}} \; .$$

10. Conclusion:

A viable organic molecule, a Class II Mesoionic Xanthine, has been introduced as a potential 10-qubit register substrate material for scalable quantum computing. We have shown that the ground state of this xanthine molecule exists in a superposition of ten unique wavefunctions. These unique wavefunctions can form the basis of 10-qubit registers for quantum computation. Additionally, a formalism was developed whereby these registers may be efficiently initialized, subsequently read into and transformed via standard unitary algorithms. We propose that polar solutions of the mesoionic xanthines or small crystalline quantum dots may be suitable for I/O techniques. Furthermore, these solutions or quantum dots may be RF-laser pulsed at a certain set of frequencies to produce a cumulative resonant interaction within the xanthines to exploit higher degrees of freedom resulting from new higher dimensional (HD) commutation rules. Relaxation of the numerous excited states via these HD commutation rules are putatively a vehicle to ontologically overcome the decoherence problem associated with QC applications [24]. This ability overcomes the major obstacle for bulk quantum computing.

References:

[1] Mbagwu, G. O., Bass, R. G. and Glennon, R. A., *J. Heterocyclic Chem.*, **22**, 465 (1985).
[2] Mbagwu, G. O., Bass, R. G. and Glennon, R. A., *Org. Magn. Reson.*, **21**, 527, (1983).
[3] Rogers, M. E., Glennon, R. A., Bass, R. G., Mbagwu, G. O., Smith, J. D., Boots, M. R., Nanavati, N., Maconaughey, J. E., Aub, D. and Thomas, S., *J. Med Chem.*, **24**, 1284 (1981).
[4] Mbagwu, G. O., *Diss. Abs. Int.,* **B42** 4428 (1982).
[5] Mbagwu, G. O., Bass, R. G. and Glennon, R. A., *Virginia J. Sci.* **31**, 113, (1980).
[6] Mbagwu, G. O., Bullock, B., and H. O., Greer, *J. Heterocyclic Chem.*, **22**, 475 (1988).
[7] Mbagwu, G. O., and Garland, R., *J. Heterocyclic Chem.*, **22**, 571 (1988).
[8] Giandinoto, S., Mbagwu, G. O., Robinson, T. A., Ferguson, C., Nunez, J., *J. Heterocyclic Chem.*, **33**, 1839 (1996).
[9] Coburn, R. A., *J. Heterocyclic Chem.*, **8**, 881 (1971).
[10] Coburn, R. A., Carapellotti, R. A., Glennon, R. A., *J. Heterocyclic Chem.*, **10**, 479 (1973).
[11] Nielsen, M. A. and Chuang, I. L., Quantum Computation and Quantum Information, Cambridge University Press, p. xxiv, Eighth Printing (2005).
[12] Nielsen, M. A. and Chuang, I. L., Quantum Computation and Quantum Information, Cambridge University Press, pp. 71-5, Eighth Printing (2005).
[13] Nielsen, M. A. and Chuang, I. L., Quantum Computation and Quantum Information, Cambridge University Press, pp. 76-8, Eighth Printing (2005).

[14] Levine, I. N., <u>Quantum Chemistry</u>, pp. 87-90, Prentice Hall, Englewood Cliffs, New Jersey, Fourth Edition (1991).

[15] Levine, I. N., <u>Quantum Chemistry</u>, p. 259, Prentice Hall, Englewood Cliffs, New Jersey, Fourth Edition (1991).

[16] Nielsen, M. A. and Chuang, I. L., <u>Quantum Computation and Quantum Information</u>, Cambridge University Press, p. 70, Eighth Printing (2005).

[17] Nielsen, M. A. and Chuang, I. L., <u>Quantum Computation and Quantum Information</u>, Cambridge University Press, pp. 98-102, Eighth Printing (2005).

[18] Nielsen, M. A. and Chuang, I. L., <u>Quantum Computation and Quantum Information</u>, Cambridge University Press, pp. 82-4, Eighth Printing (2005).

[19] Nielsen, M. A. and Chuang, I. L., <u>Quantum Computation and Quantum Information</u>, Cambridge University Press, pp. 174-5, Eighth Printing (2005).

[20] Ventura, D. and Martinez, T., *Found. Phys. Lett.,* **12**, 547 (1999).

[21] Gui-Lu Long and Yang Sun, "Efficient Scheme for Initializing a Quantum Register with an Arbitrary Superposed State", arXiv:quant-ph/0104030v1 (2007).

[22] Barenco, A., *et. al., Phys. Rev.* **A52**, 3457 (1995);Barenco, A., *Proc. R. Soc. London,* **A449**, 679 (1995).

[23] Grover, L. K., *Phys. Rev. Lett.,* **79**, 325 (1997).

[24] Amoroso, R.L., Giandinoto, S., Hunter, G., Nibart, G., & Rauscher, E.A., Universal Quantum Computing: Anticipatory Parameters Predicting Bulk Implementation, *Part 1-Philosophical Foundations for the Formalism*, in D. Dubois (ed.) Proceedings of CASYS'07, Liege, Belgium.