Concept of chemical bond and aromaticity based on quantum information theory

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Quantum information theory (QIT) emerged in physics as standard technique to extract relevant information from quantum systems. It has already contributed to the development of novel fields like quantum computing, quantum cryptography, and quantum complexity. This arises the question what information is stored according to QIT in molecules which are inherently quantum systems as well. Rigorous analysis of the central quantities of QIT on systematic series of molecules offered the introduction of the concept of chemical bond and aromaticity directly from physical principles and notions. We identify covalent bond, donor-acceptor dative bond, multiple bond, charge-shift bond, and aromaticity indicating unified picture of fundamental chemical models from ab initio.

Extension of information theory¹ for quantum systems, called quantum information theory (QIT)²–¹, leads to emergence of non classical correlations, entanglement. In the past decade various concepts of QIT have matured to widely used tools in quantum many body physics. Several well known quantities have been redefined in term of entanglement shedding new light in our understanding of quantum systems.

In chemistry such concepts have appeared only recently⁷–¹⁰ although correlations among components of a finite system, like orbitals, can be regarded as exchanging information among such parties. For example, single orbital entropy provides information about how much an orbital is entangled with the rest of the system. In addition, two-orbital mutual information¹¹,¹² determines how orbitals communicate with each other, i.e., it gives the correlation between two orbitals as they are embedded in the whole system. The mutual information, however, contains correlations of both classical and quantum origin.¹³ Such central quantities to describe orbital correlations have already been applied recently by some of us to analyze copper-oxide clusters¹⁴ to dissect electron correlation effects in bond-forming and bond-breaking processes.¹⁵,¹⁶,¹⁸ In addition, entanglement structures have also been determined in photosystem II¹⁹ and orbital entanglement analysis of the Ru–NO bond in a Ruthenium nitrosyl complex has also been carried out.²⁰ In all these works, correlations among the orbitals were measured in terms of quantum information entropies which are weighted averages of the eigenvalue spectrum of the various subsystem density matrices (see Eq. (1)). Therefore, the more detailed information encoded in the the eigenvalue spectrum²¹,²² and in the structure of the corresponding eigenstates of reduced density matrix has been lost.

In this work, we present a systematic analysis of (multi-)orbital entanglement together with the probability distribution of eigenstates given by the corresponding reduced density matrices for all possible realizations of the two-orbital subsystems in series of handful of molecules. As a result, we find strong connection between our approach and basic chemical models which allow us to describe covalent bonds, donor-acceptor dative bonds, multiple bonds, charge-shift bond, and aromaticity from a unified point of view.

Theoretical background: When a system is split into two parts called a bipartite system (the two parts often called Alice and Bob), the Hilbert space is \(\mathcal{H} = \mathcal{H}^A \otimes \mathcal{H}^B\). If the system can be described by a pure state, the wave function is a linear combination of the tensor product of the basis functions of the two subsystems \(\langle \phi_{AB}^{(A)} | \phi_{AB}^{(B)} \rangle\), i.e., \(\Psi = \sum_{\alpha\beta} C_{\alpha\beta} |\phi_{\alpha}(A)\rangle \otimes |\phi_{\beta}(B)\rangle\), where \(C_{\alpha\beta}\) is a complex matrix in general. The correlations between the two subsystems is fully quantum and called entanglement. The wave function can also be written as a single sum of the product of transformed basis states due to Schmidt decomposition, i.e., \(\Psi = \sum_{\alpha=1}^{r} \sqrt{\omega_{\alpha}} |\xi_{\alpha}(A)\rangle \otimes |\xi_{\alpha}(B)\rangle\), where \(r \leq \min(\dim \mathcal{H}^A, \dim \mathcal{H}^B)\), \(\omega_{\alpha} \geq 0\), and \(\sum_{\alpha=1}^{r} \omega_{\alpha} = 1\). The square of the \(\sqrt{\omega_{\alpha}}\) Schmidt values are also equal to the eigenvalues of the so-called reduced density matrix, \(\rho^{(A)}\), formed by tracing out one subsystem², i.e., \(\rho^{(A)} = \text{Tr}_B |\Psi\rangle \langle \Psi|\), thus \(\rho_{\alpha\alpha'}^{(A)} = \sum_{\beta} C_{\alpha\beta} C_{\alpha'\beta}^{*} |\xi_{\alpha}(A)\rangle \langle \xi_{\alpha'}(A)|\) and \(|\xi_{\alpha}(A)\rangle\) are the eigenstates of \(\rho^{(A)}\) and \(\rho^{(B)}\), respectively. If \(r = 1\) the wave function \(|\Psi\rangle\) is a product state and the system is called separable, otherwise it is said to be entangled.

In general, both subsystems are in a mixed state and the total system cannot be written as a single product of the states of the two subsystems. There are various quantities introduced to measure the mixedness of the subsystems and the strength of entanglement but they all must fulfill an important criterion namely entanglement monotonicty²³–²⁵. This means that the quantity cannot increase by local operations and classical communication (LOCC). A widely used quantity is the entanglement entropy given by the von-Neumann entropy of the reduced density matrix calculated as

\[
S(\rho^{(A)}) = -\sum_{\alpha} \omega_{\alpha}^{(A)} \ln \omega_{\alpha}^{(A)}.
\]

There are various possibilities to split a system into two or several subsystems. If subsystem \((A)\) contains...
a single orbital and subsystem (B) the rest of the orbitals, the single-orbital entropy, $S(\rho(i))$, can be calculated with $i = 1, \ldots, N$, where $N$ is the number of orbitals. Assuming four basis states per orbital, i.e., $|\phi(i)\rangle \in \{|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle\}$, the theoretical maximum of $S(\rho(i))$ is $\ln 4$ with $\omega_\alpha = 1/4$ for all $\alpha = 1, \ldots, 4$.

The correlation between two orbitals, $i$ and $j$, as they are embedded in the whole system is given by the two-orbital mutual information $I(i,j)$

$$I(i,j) = S(\rho(i)) + S(\rho(j)) - S(\rho(i,j))$$

where $S(\rho(i))$, $S(\rho(j))$, and $S(\rho(i,j))$ are the single-orbital and two-orbital entropies, respectively. In this case $\rho(i,j)$ is also a mixed state thus the mutual information contains correlations of both classical and quantum origin.

An eigenvalue of $\rho(i,j)$ denoted by $\omega_\alpha(i,j)$ corresponds to eigenvector $|\phi_\alpha(i,j)\rangle = \sum_\alpha C_{\alpha\alpha}(i,j) |\alpha\rangle \otimes |\alpha\rangle$ where $\alpha_i$ and $\alpha_j$ run from 1 to 4 and $\alpha = 1, \ldots, 16$. Again the theoretical maximum of $I(i,j) = \ln 16$ corresponds to maximally entangled pure two-orbital state with $\omega_\alpha = 1/4$ for all $\alpha$ and $S(\rho(i)) = S(\rho(j)) = \ln 4$, but orbital pair state (i, j) is in a pure state with $S(\rho(i,j)) = 0$.

In case of quantum chemical systems for the number of electrons are correlated on finite number of orbitals and the number of electrons, $n$, as well as the total spin projection, $s^z$, are good quantum numbers. $\rho(i,j)$ also commute with the Hamilton operator and it has a block diagonal structure and the $\alpha$th eigenstate of the two-orbital subsystem with quantum number pair $(n, s^z)$ (with $n = 0, \ldots, 4$ and $s^z \in \{-1, -1/2, 0, 1/2, 1\}$ can be written as a linear combinations of basis states in the corresponding subspace. The set of $c_{\alpha\alpha}(i,j)$ coefficients corresponding to basis states with quantum number pair $(n, s^z)$ will be labeled by a vector $c(i,j)(n, s^z)$ in order to use a compact notation for the rest of the paper. Therefore, $c(i,j)(0,0)$ corresponds to $|0\rangle, |\downarrow\rangle$, $c(i,j)(1, -\frac{1}{2})$ to $|\uparrow\rangle, |\downarrow\rangle$, $c(i,j)(1, \frac{1}{2})$ to $|\uparrow\rangle, |\uparrow\rangle$, $c(i,j)(2, 0)$ to $\{|0\uparrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\rangle\}$, $c(i,j)(2, -1)$ to $|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle$, $c(i,j)(2, 1)$ to $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$, $c(i,j)(3, -\frac{1}{2})$ to $\{|\uparrow\uparrow\rangle, |\downarrow\rangle, |\downarrow\rangle\}$, $c(i,j)(3, \frac{1}{2})$ to $\{|\uparrow\downarrow\rangle, |\uparrow\rangle, |\uparrow\rangle\}$, and $c(i,j)(4, 0)$ to $\{|\uparrow\rangle, |\uparrow\rangle\}$.

In the rest of the paper, $\omega(i,j)$ eigenvalues will be ordered decreasingly, i.e., the largest value will correspond to $\alpha = 1$ and the smallest to $\alpha = 16$. We will use the term relevant eigenvalue if it is one or two orders of magnitude larger than the remaining ones. The elements of the $c(i,j)(n, s^z)$ vector will be given in terms of its largest element in order to show the ratio among the coefficients. Furthermore, in some cases the equality among the various $c(i,j)(n, s^z)$ vectors discussed in the next section will hold up to a spin reversal.

Results and Discussion

Fig. 1 shows the mutual information results of eight small molecules, BH$_3$, CH$_4$, NH$_3$, H$_2$O, HF, F$_2$, N$_2$, and CO. Numbers on each pictures only refer to different sites which orbitals are also shown around. Mutual information is indicated by the color of the lines between the sites. The lack of strong visible line between sites is the sign of negligible communication; these orbital correlations do not contain relevant information. The maximum of the mutual information is marked by the theoretical limit, $I_{\text{limit}} = 2.77$, as it was discussed earlier.

The mutual information analysis of BH$_3$ reveals three strong entanglements given by $I(1,6) = I(3,7) = I(4,8) = 2.68$ (Fig. 1a). All other 25 possible connections are zero within numerical accuracy. Therefore, site #2 and #6 do not communicate with other sites which is in accordance with the chemical insight as site #2 is the inert 1s core orbital while site #6 is the empty $2p$ orbital of the boron. The calculated mutual information of the correlated sites are identical and very close to the theoretical upper limit as their two-orbital reduced density matrix is dominated by a single eigenvalue $\omega_1 = \omega_{3,7} = \omega_{4,8} \approx 0.992$. In the corresponding eigenvector, elements $|0\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\rangle, |\downarrow\rangle, |\downarrow\rangle, |\downarrow\rangle, |\downarrow\rangle, |\downarrow\rangle$, have almost the same relevance in the description of the interaction, i.e., $c_1^{(1,5)}(2,0) = c_1^{(3,7)}(2,0) = c_1^{(4,8)}(2,0) = 0.541 \times 0.80, -1, 1, 0.88$. Mutual information analysis of other small molecules like NH$_3$, H$_2$O, HF, and F$_2$ (Fig. 1c-f) shows similar overall picture to BH$_3$ and CH$_4$ indicating 3, 2, 1, and 1 very strong mutual information between sites, respectively (see also in SI I). These correlations always connect orbitals on different atoms and thus can be assigned to chemical bonds. The calculated mutual information of NH$_3$, H$_2$O, HF, and F$_2$ is, however, only 2.52, 2.23, 1.85, and 1.47 smaller for these correlations than that in the case of BH$_3$ and CH$_4$. Deviation from the theoretical limit reflects the relative difference of the elements of the eigenvector and the presence of additional correlations of sites. For NH$_3$, one eigenvalue dominates $\omega_1 = \omega_2 = \omega_{5,8} = 0.967$ with moderate difference in the weight of the eigenvector elements, $c_1^{(1,6)}(2,0) = c_1^{(2,7)}(2,0) = c_1^{(5,8)}(2,0) = 0.541 \times 0.73, -1, 1, 0.94$. For H$_2$O, the eigenvector elements have even more asymmetric distribution compared to NH$_3$ ($c_1^{(1,6)}(2,0) = c_1^{(5,7)}(2,0) = 0.539 \times 0.69, -1, 1, 0.98$).

Besides, site #4, the lone pair in the plane, has also minor contribution to the mutual information picture, $I(1,6) = I(3,7) = I(4,8) = 0.22$. These values are one order of magnitude smaller than the
FIG. 1. Graphical representation of mutual information for basic small molecules: BH$_3$ (a), CH$_4$ (b), NH$_3$ (c), H$_2$O (d), HF (e), F$_2$ (f), N$_2$ (g), and CO (h). The color of the bonds according to the color scale (i) indicates the mutual information of the connected two sites. The shape of the molecular orbitals (isovalue 0.05) are shown directly near the sites. The blue and red colors of the orbitals refer to the sign of the wave function. Atoms are labeled with their usual colors; H, B, C, N, O, and F atoms marked with white, brown, tan, blue, red, and purple colors, respectively.

usual ones $I^{(1,6)} = I^{(5,7)} = 2.23$. Further analysis reveals that this secondary effect comes from the three electron regime given by the second largest eigenvalue, $\omega^{(4,6)}_2 = 0.249$ and the corresponding vector elements of $c^{(4,6)}(3, \pm \frac{1}{2})$. These secondary correlations are present between a site with two electrons and the two sites with large mutual information which may be regarded as hyperconjugative effect between a lone pair and an adjacent bond. Similar effects are observed for HF and F$_2$ as well which is also partly responsible for the lower value of $I$ which is assigned to the chemical bond. However, the main reason is the large value of the second largest eigenvalue. For HF, $\omega^{(1,6)}_2 = \omega^{(1,6)}_3 = 0.118$, while for F$_2$ $\omega^{(5,10)}_2 = \omega^{(5,10)}_3 = 0.174$. It turns out that this second and third eigenvalues are associated with the three-electron regime. For HF, $c^{(1,6)}_2(3, \pm \frac{1}{2}) = c^{(1,6)}_3(3, \pm \frac{1}{2}) = 0.882 \times [1, -0.53]$, for F$_2$ $c^{(5,10)}_2(3, \pm \frac{1}{2}) = c^{(5,10)}_3(3, \pm \frac{1}{2}) = 0.707 \times [1, 1]$. It formally means that an extra electron resonates between the two sites which is consistent with picture of charge-shift bond.$^{28,29}$ The orbital pictures of Fig. 1 underline this correspondence.

Multiple bonds: We investigate N$_2$ and CO as model compounds for multiple bond systems (Fig. 1g, h). Indeed, the mutual information analysis results in three bonds for both molecules as expected but detailed investigation identify fundamental differences. For $\pi$-bond in N$_2$, the eigenvector elements, $c^{(5,8)}_1(2,0) =$
FIG. 2. Graphical representation of mutual information for the series of NH$_3$BH$_3$ (a), NH$_2$BH$_2$ (b), NHBH (c), CH$_3$CH$_3$ (d), CH$_2$CH$_2$ (e), CHCH (f), SiH$_3$CH$_3$ (g), SiH$_2$CH$_2$ (h), and SiHCH (i). The color of the bonds indicates the mutual information of the connected two sites. The shape of the important molecular orbitals (isovalue 0.05) are shown on the two sides where numbers near the orbitals indicate the site number. The blue and red colors of the orbitals refer to the sign of the wave function. Atoms are labeled with their usual colors; H, B, C, N, and Si atoms marked with white, brown, tan, blue, and yellow colors, respectively.

$e_{1}^{(3,10)}(2,0) = 0.573 \times [0.72, 1, -1, 0.72]$, are similar to the previously discussed covalent bonds with the dominance of electron-sharing components. While the $\pi$ bonds of CO, however, have strong asymmetric distribution in eigenvector elements, $e_{1}^{(5,8)}(2,0) = e_{1}^{(4,9)}(2,0) = 0.644 \times [0.36, 0.80, -0.80, 1]$, which surpass the usual asymmetry resulted from the polarization of the bond. Therefore, we conclude that QIT analysis may be able to differentiate between covalent and donor-acceptor bonds as well.

Dative and multiple bonds: Unfortunately, owing to the symmetry of the CO molecule we cannot examine separately the two $\pi$ bonds (one covalent and one donor-acceptor bonds) and support our hypothesis. To gain deeper insight, we investigate a series of molecules which can help to elucidate this question. We choose NH$_3$BH$_3$, NH$_2$BH$_2$, and NHBH for donor-acceptor test systems; CH$_3$CH$_3$, CH$_2$CH$_2$, and CHCH for isoelectronic apolar covalent reference systems. We also calculate SiH$_3$CH$_3$, SiH$_2$CH$_2$, and SiHCH as polarized covalent analogs which also serve as an example for bonds containing heavier element (see Fig. 2). In the rest of the paper, we only focus on the newly emerged bonding modes, while the previously discussed bond types are considered as known, if it is not mentioned otherwise. As an example, in this section, all C-H, N-H, and B-H bonds show similar picture as we have discussed for these type of bonds in the case of BH$_3$, CH$_4$, and NH$_3$. We note that this result also indicates that QIT based analysis is robust, yields the same relevant information for the same chemical moiety. We provide all details for all investigated molecules in Supporting Information II.

QIT analysis for NH$_3$BH$_3$ (Fig. 2a) provides the similar results to the donor-acceptor bond of CO. The mutual information of the donor-acceptor bond is significantly lower than for the covalent bond, $I^{(5,13)} = 1.75$. The eigenvector elements show drastic asymmetric distribution and the weight of electron-sharing parts is also smaller than in the previous examples: $e_{1}^{(5,13)}(2,0) = 0.762 \times [0.23, -0.58, 0.58, 1]$. For the isoelectronic analog CH$_3$CH$_3$ (Fig. 2d), the C-C bond, site #5 and #13, has similar values to other covalent bonds; $I^{(5,13)} = 2.49$, the eigenvector elements indicate difference from donor-acceptor bonding mode $e_{1}^{(5,13)}(2,0) = 0.542 \times [0.84, 1, -1, 0.84]$. SiH$_3$CH$_3$ with polarized Si-C covalent bond shows the expected results (Fig. 2g); mutual information is larger ($I^{(17,18)} = 2.28$) than that of the
FIG. 3. Graphical representation of mutual information for the series of delocalized systems: \( \text{CH}_2\text{CHBH}_2 \) (a), \( \text{CH}_2\text{CHNH}_2 \) (b), butadiene (c), cyclobutadiene (d), borole (e), benzene (f), pyrrole (g), furan (h), and thiophene (i). The color of the bonds indicates the mutual information of the connected two sites. The shape of the important molecular orbitals (isovalue 0.05) are shown on the two sides where numbers near the orbitals indicate the site number. The blue and red colors of the orbitals refer to the sign of the wave function. Atoms are labeled with their usual colors; H, B, C, N, O, and S atoms marked with white, brown, tan, blue, red, and yellow colors, respectively.

donor-acceptor analog but somewhat smaller than that of the homonuclear analog. The important eigenvector elements show the expected asymmetry \( c_{1}^{17,18}(2,0) = 0.553 \times [1, -0.96, 0.96, 0.64] \). Such direct comparison can be flawed by the large electronegativity difference of atoms therefore we investigate \( \text{NH}_2\text{BH}_2 \). The mutual information analysis suggests two strong interactions between N and B atoms (Fig. 2b), \( I^{(3,4)} \) and \( I^{(6,11)} \), in accordance with the double bond structure. Interestingly, the QIT results of these bonds are quite different. On one hand, \( I^{(3,4)} = 2.38 \) close to the values of previously mentioned covalent bonds and the eigenvector elements of the largest \( \omega^{(3,4)} \) also supports the polarized covalent bond assignment based on previous examples \( c_{1}^{3,4}(2,0) = 0.628 \times [1, 0.80, -0.80, 0.51] \). On the other hand, \( I^{(6,11)} = 1.94 \) is much lower and the eigenvector elements is determined by the strongly asymmetric distribution \( c_{1}^{6,11}(2,0) = 0.768 \times [0.16, 0.58, -0.58, 1] \) similar to the donor-acceptor dative bond in \( \text{NH}_3\text{BH}_3 \).

Assignation based on orbital images proves that the aforementioned results are consistent with the chemical picture; the \( \pi \) bond is the dative bond while the \( \sigma \) is the covalent bond in \( \text{NH}_2\text{BH}_2 \). Although, these results indicate no clear cut between covalent and dative bonds but the difference is prominent which is enough to assign them even within a double bond. Analog molecules \( \text{CH}_2\text{CH}_2 \) (Fig. 2e) and \( \text{SiH}_2\text{CH}_2 \) (Fig. 2h) show the expected results indicating covalent bonds; \( I^{(2,3)} \) for these four bonds is in the range of 2.3-2.5 (see details in Supporting Information II E, II H). For \( \text{NHBH} \) (Fig. 2c), a sigma bond is given by \( I^{(2,3)} = 2.48, c_{1}^{(2,3)}(2,0) = 0.602 \times [1, 0.84, -0.84, 0.60] \), while the two \( \pi \) bonds are identical, because of symmetry reasons \( I^{(5,9)} = I^{(6,10)} = 1.91, c_{1}^{(5,9)}(2,0) = c_{1}^{(6,10)}(2,0) = 0.644 \times [0.35, 0.80, -0.80, 1] \). These results are nearly the same as the results of CO suggesting the same bonding mode. For analog \( \text{CHCH} \) (Fig. 2f), we obtain almost the same results as for \( \text{N}_2 \); for the \( \sigma \) bond: \( I^{(2,3)} = \)
Aromaticity: Molecules with cyclic delocalization have a special place in chemists’ mind as the subject of the concept of aromaticity and antiaromaticity. Therefore, we extended our investigation to this direction. From butadiene and hexatriene one can derive the prototype antiaromatic and aromatic systems, cyclobutadiene and benzene (Fig. 3c and 3e, respectively, and in SI IV and V). For cyclobutadiene, mutual information analysis indicates two strong correlations in the $\pi$-system, $I(\pi) = I(12,22) = 2.33$. Interestingly, the secondary effects observed in butadiene is disappeared in cyclobutadiene. We have not found any communication between the $\pi$-subsystems within numerical accuracy, only the $\sigma$-system show some minor effects probably due to their strained structure. Another antiaromatic compound butadiene shows the similar effects (Fig. 3c). In the $\pi$-system two C-C moiety are found, similar to CH$_2$CH$_2$BH$_2$. However, there is no secondary effect in the butadiene moiety. Opposite effects can be seen for benzene. The strong mutual information between C-C $\pi$-bonds become less dominant while secondary effects are even stronger compared to hexatriene and thus a cyclic structure is seen in the mutual information picture with very low value $I(\pi) = I(19,15) = I(26,30) = 0.18$, indicating their direct relationship. We have also investigated the aromatic series of furan, pyrrole, and thiophene (Fig. 3g-i). Interestingly, five-membered cyclic structure dominates the mutual information picture of the pyrrole molecule which is in wide contrast to borole. The secondary effects increased between butadiene moiety while the CH$_3$CH$_2$NH$_2$ structure is less emphasized. Cyclic delocalization with reduced mutual information between C-C double bonds and increased secondary correlations are found for furan and thiophene as well indicating similar effects to benzene and pyrrole. In the mutual information picture of furan and thiophene an additional weak structure is also found which are the hyperconjugative interaction of the lone pair with the adjacent $\sigma$-bonds similar to what has been found for water.

In conclusion, we have introduced a novel approach to extract information from molecules based on QIT analysis. Systematic investigation of handful of molecules using localized orbitals offers the introduction of the concept of chemical bond and aromaticity. We have shown on several examples how different chemical models like covalent bond, donor-acceptor dative bond, multiple bond, charge-shift bond, conjugation, and aromaticity follows from QIT. The discussed results indicate the unified picture of chemical concepts and therefore can help to elucidate their fundamental features and may lead to an improved definition of chemical bond. This study also closes the gap between state-of-the-art physical and traditional chemical models showing their mutual origin. Although there are many open questions regarding the QIT analysis of molecules we envision that our approach can be used in the future alternatively or together with well known chemical bond analysis methods$^{30-34}$ and elucidate unique bonding modes.$^{35,36}$

Methods

In this paper we have performed numerical calculations using the quantum chemistry version of the density matrix renormalization group (QC-DMRG) method.$^{37,38}$ We have controlled the numerical accuracy using the dynamic block state selection (DBSS) approach$^{39}$ and the maximum number of block states varied in the range of 500-2000 for an a priori set quantum information loss threshold value $\chi = 10^{-5}$. The ordering of molecular orbitals along the one-dimensional topology of the DMRG was optimized using the Fiedler approach$^{14,17}$ and the active space was extended dynamically based on the dynamically extended active space (DEAS) procedure. We have controlled the numerical accuracy using the dynamic block state selection (DBSS) approach$^{39}$ and the maximum number of block states varied in the range of 500-2000 for an a priori set quantum information loss threshold value $\chi = 10^{-5}$. The ordering of molecular orbitals along the one-dimensional topology of the DMRG was optimized using the Fiedler approach$^{14,17}$ and the active space was extended dynamically based on the dynamically extended active space (DEAS) procedure. We have controlled the numerical accuracy using the dynamic block state selection (DBSS) approach$^{39}$ and the maximum number of block states varied in the range of 500-2000 for an a priori set quantum information loss threshold value $\chi = 10^{-5}$. The ordering of molecular orbitals along the one-dimensional topology of the DMRG was optimized using the Fiedler approach$^{14,17}$ and the active space was extended dynamically based on the dynamically extended active space (DEAS) procedure. We have controlled the numerical accuracy using the dynamic block state selection (DBSS) approach$^{39}$ and the maximum number of block states varied in the range of 500-2000 for an a priori set quantum information loss threshold value $\chi = 10^{-5}$. The ordering of molecular orbitals along the one-dimensional topology of the DMRG was optimized using the Fiedler approach$^{14,17}$ and the active space was extended dynamically based on the dynamically extended active space (DEAS) procedure. We have controlled the numerical accuracy using the dynamic block state selection (DBSS) approach$^{39}$ and the maximum number of block states varied in the range of 500-2000 for an a priori set quantum information loss threshold value $\chi = 10^{-5}$. The ordering of molecular orbitals along the one-dimensional topology of the DMRG was optimized using the Fiedler approach$^{14,17}$ and the active space was extended dynamically based on the dynamically extended active space (DEAS) procedure.
of theory which yielded sufficient geometries in accordance with higher level methods. In QIT, we are especially interested in the communication of subsystems which may communicate through active sites belonging to different subsystems. In molecules, atoms seem a natural choice for the definition of subsystem. To create sites which correspond to one atom, we have applied localized orbitals as sites. We have chosen Piek-Pekey procedure with tight threshold $10^{-12}$ and minimized the number of atomic orbitals contributed in each localized orbitals. Therefore, they can be easily identified as part of a subsystem and because of the minimal basis set their chemical meaning is also clear which we can use for later comparison. All localized orbitals have been used in the DMRG procedure thus, as a result, we have carried out calculations at the FCI limit for all molecules. Then, results at the FCI limit have been analyzed in the paper. All preliminary calculations have been done by MOLPRO Version 2010.141.

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Supplemental Materials: Concept of chemical bond and aromaticity based on quantum information theory

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In the Supporting Information (SI) we present the graphical representation of the single-site entropy $S(\rho^{(i)})$ and the corresponding $\omega_\alpha^{(i)}$ eigenvalue spectrum ($\alpha = 1 \ldots 4$) as a function of orbital index $(i)$. Furthermore, we show pair-wise elements of the two-orbital mutual information ($I^{(i,j)}$) indicated by the color of the lines between the sites. The lack of strong visible line between sites is the sign of negligible communication; these orbital correlations do not contain relevant information. The maximum of the mutual information is marked by the theoretical limit, $\ln 16 \approx 2.77$. The largest $\omega_\alpha^{(i,j)} > 0.1$ eigenvalues of the corresponding two-orbital reduced matrix $\rho^{(i,j)}$ are collected in a table format together with the eigenvector coefficients obtained in the different quantum number sectors of the two-site subsystem.

I. MOLECULES WITH COVALENT BONDS

A. BH$_5$

| i | j | $I^{(i,j)}$ | $\omega_\alpha$ | $n = 2$, $s^z = 0$ |
|---|---|---|---|---|
| 4 | 8 | 2.679 | 0.992 | -0.431 -0.541 0.541 -0.477 |
| 1 | 5 | 2.679 | 0.992 | -0.431 -0.541 0.541 -0.477 |
| 3 | 7 | 2.679 | 0.992 | -0.431 -0.541 0.541 -0.477 |
B. CH₄

\[
\begin{array}{cccc}
1 & 8 & 2.682 & 0.993 \\
2 & 7 & 2.682 & 0.993 \\
3 & 9 & 2.682 & 0.993 \\
4 & 5 & 2.682 & 0.993 \\
\end{array}
\]

\[
\begin{array}{cccc}
\uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow \\
-0.430 & -0.543 & 0.543 & 0.474 \\
0.430 & -0.430 & -0.543 & 0.543 \\
0.543 & 0.543 & -0.474 & -0.474 \\
\end{array}
\]
C. NH$_3$

\begin{center}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & $\omega_{ij} > 0.1$ & $\n = 2$, $s^z = 0$ \\
\hline
1 & 6 & 2.524 & 0.967 & \text{not } \uparrow \downarrow & \text{not } \uparrow \downarrow & \text{not } \uparrow \downarrow & \text{not } \uparrow \downarrow \\
5 & 8 & 2.524 & 0.967 & 0.397 & -0.541 & 0.541 & 0.506 \\
2 & 7 & 2.524 & 0.967 & 0.397 & -0.541 & 0.541 & 0.506 \\
\hline
\end{tabular}
\end{center}
D. \text{H}_2\text{O}

\[
\begin{array}{cccccc}
\text{i} & \text{j} & l(i,j) & \omega_{l(i)} > 0.1 & n = 2, s^z = 0 & n = 3, s^z = 1/2 & n = 4, s^z = 1/2 \\
5 & 7 & 2.226 & 0.889 & -0.371 & -0.530 & -0.539 \\
1 & 6 & 2.226 & 0.889 & -0.371 & -0.530 & -0.539 \\
4 & 6 & 0.302 & 0.302 & 0.031 & 0.360 & 0.360 \\
4 & 7 & 0.302 & 0.302 & -0.031 & 0.360 & -0.360 \\
4 & 5 & 0.218 & 0.136 & 0.026 & 0.291 & -0.291 \\
1 & 4 & 0.218 & 0.136 & -0.011 & 0.291 & -0.291 \\
\end{array}
\]
E. HF

| i | j | I(i,j) | $\omega_{\alpha} > 0.1$ | $n = 2, s^z = 0$ |
|---|---|--------|----------------|----------------|
| 1 | 6 | 1.854  | 0.760 0.823 0.528 0.528 0.581 |
| 5 | 6 | 0.498  | 0.353 0.037 -0.369 0.369 0.852 |
| 1 | 5 | 0.396  | 0.107 0.861 0.357 -0.357 0.067 |
| 4 | 6 | 0.283  | 0.303 0.005 -0.277 0.277 0.920 |
| 3 | 6 | 0.230  | 0.292 -0.001 -0.248 0.248 0.936 |

| i | j | I(i,j) | $\omega_{\alpha} > 0.1$ | $n = 0$ | $n = 3, s^z = -1/2$ | $n = 3, s^z = 1/2$ | $n = 4$ |
|---|---|--------|----------------|--------|----------------|----------------|--------|
| 1 | 6 | 1.854  | 0.118 0.000 -0.000 0.000 0.882 -0.470 0.000 |
| 6 | 1 | 0.488  | 0.271 0.000 0.072 0.234 0.000 0.000 0.000 |
| 1 | 5 | 0.396  | 0.274 0.000 -0.000 0.000 0.424 -0.906 0.000 |
| 5 | 1 | 0.345  | 0.274 0.000 -0.000 0.000 0.000 0.000 1.000 |
| 4 | 6 | 0.283  | 0.288 0.000 0.987 0.161 -0.000 -0.000 0.000 |
| 6 | 4 | 0.233  | 0.256 0.000 -0.000 0.000 0.307 -0.352 0.000 |
| 4 | 1 | 0.230  | 0.292 0.000 0.000 0.000 0.990 0.141 0.000 |
| 1 | 4 | 0.191  | 0.252 0.000 0.273 -0.962 -0.000 0.000 0.000 |
| 3 | 5 | 0.124  | 0.813 0.000 0.000 0.000 0.000 0.000 1.000 |
| 5 | 3 | 0.106  | 0.827 0.000 0.000 0.000 0.000 0.000 1.000 |
\[ F \quad F_2 \]

\[ I(i,j) \quad \omega_\alpha > 0.1 \]

\[ \begin{array}{cccccc}
5 & 10 & 1.469 & 0.583 & -0.422 & 0.568 & -0.568 & -0.422 \\
1 & 10 & 0.704 & 0.158 & 0.119 & -0.407 & 0.407 & 0.609 \\
5 & 9 & 0.699 & 0.158 & 0.810 & -0.406 & 0.406 & 0.117 \\
1 & 5 & 0.582 & 0.236 & 0.097 & -0.525 & 0.525 & 0.663 \\
9 & 10 & 0.578 & 0.234 & 0.096 & -0.524 & 0.524 & 0.665 \\
\end{array} \]
### N₂

#### Table 1: Orbital Index

| i | j | I(i,j) | ω_α > 0.1 | n = 2, s^z = 0 | n = 3, s^z = -1/2 | n = 3, s^z = 1/2 | n = 4 |
|---|---|---|---|---|---|---|---|
| 4 | 9 | 0.216 | 0.865 | -0.48 | -0.517 | 0.177 | -0.482 |
| 5 | 8 | 0.201 | 0.857 | -0.415 | 0.573 | 0.573 | -0.415 |
| 3 | 10 | 0.201 | 0.857 | -0.415 | -0.573 | 0.573 | -0.415 |
| 3 | 5 | 0.251 | 0.229 | -0.291 | -0.644 | 0.644 | -0.291 |
| 8 | 10 | 0.251 | 0.229 | 0.291 | -0.644 | 0.644 | 0.291 |
| 7 | 9 | 0.247 | 0.229 | -0.027 | 0.234 | -0.234 | 0.943 |
| 4 | 7 | 0.247 | 0.229 | 0.027 | 0.234 | -0.234 | 0.943 |
| 4 | 7 | 0.229 | 0.233 | 0.255 | 0.255 | 0.255 | 0.943 |
| 7 | 9 | 0.229 | 0.233 | -0.023 | 0.285 | -0.285 | -0.932 |

#### Diagram 1: Orbital Probability Density

| i | j | I(i,j) | ω_α > 0.1 | n = 0 | n = 3, s^z = -1/2 | n = 3, s^z = 1/2 | n = 4 |
|---|---|---|---|---|---|---|---|
| 7 | 9 | 0.247 | 0.266 | 0.000 | 0.968 | 0.252 | 0.000 |
| 8 | 9 | 0.233 | 0.000 | 0.000 | 0.000 | -0.223 | 0.975 |
| 1 | 4 | 0.247 | 0.266 | 0.000 | 0.000 | 0.000 | 0.968 |
| 5 | 8 | 0.233 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 |
| 4 | 7 | 0.229 | 0.259 | 0.000 | -0.223 | 0.975 | 0.000 |
| 5 | 8 | 0.240 | 0.000 | 0.000 | 0.000 | -0.223 | 0.975 |
| 1 | 9 | 0.229 | 0.259 | 0.000 | 0.000 | 0.000 | 0.968 |
H. CO

\begin{center}
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
\textbf{i} & \textbf{j} & \textbf{I(i,j)} & \textbf{\omega_{ij} > 0.1} & \textbf{n = 2, s^z = 0} & \textbf{n = 3, s^z = -1/2} & \textbf{n = 3, s^z = 1/2} & \textbf{n = 4} \\
\hline
5 & 8 & 2.194 & 0.950 & -0.230 & 0.516 & -0.516 & -0.644 \\
4 & 9 & 2.194 & 0.950 & -0.230 & 0.516 & -0.516 & -0.644 \\
3 & 10 & 2.115 & 0.863 & 0.358 & 0.502 & 0.502 & 0.606 \\
1 & 10 & 0.259 & 0.349 & 0.024 & 0.115 & -0.215 & -0.983 \\
7 & 10 & 0.251 & 0.355 & -0.020 & 0.224 & -0.224 & -0.948 \\
3 & 7 & 0.221 & 0.131 & 0.930 & 0.257 & -0.257 & 0.041 \\
1 & 3 & 0.196 & 0.136 & 0.032 & -0.297 & 0.297 & 0.907 \\
\hline
\end{tabular}
\end{center}
II. DATIVE SYSTEMS

A. NH$_3$BH$_3$

| i | j | \( l(i,j) \) | \( \omega_{\alpha} > 0.1 \) |
|---|---|---|---|
| 1 | 4 | 2.579 | 0.977 | -0.402 | -0.540 | 0.540 | -0.506 |
| 2 | 10 | 2.579 | 0.977 | -0.402 | -0.540 | 0.540 | -0.506 |
| 3 | 11 | 2.579 | 0.977 | -0.402 | -0.540 | 0.540 | -0.506 |
| 7 | 12 | 2.499 | 0.971 | -0.358 | 0.537 | -0.537 | -0.547 |
| 9 | 16 | 2.499 | 0.971 | -0.358 | 0.537 | -0.537 | -0.547 |
| 8 | 15 | 2.499 | 0.971 | -0.358 | 0.537 | -0.537 | -0.547 |
| 5 | 13 | 1.754 | 0.918 | -0.175 | 0.441 | -0.441 | -0.762 |

\( n = 2, \ s^* = 0 \)
B. \text{NH}_2\text{BH}_2

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
i & j & 1(i,j) & \omega_\alpha > 0.1 & n = 2, s^z = 0 & \\
\hline
1 & 9 & 2.591 & 0.978 & 0.120 & -0.540 & 0.540 & 0.490 & \\
2 & 10 & 2.591 & 0.978 & 0.120 & -0.540 & 0.540 & 0.490 & \\
8 & 14 & 2.534 & 0.973 & 0.379 & -0.538 & 0.538 & 0.527 & \\
7 & 13 & 2.534 & 0.973 & 0.379 & -0.538 & 0.538 & 0.527 & \\
3 & 4 & 2.377 & 0.962 & 0.628 & 0.501 & -0.501 & 0.323 & \\
6 & 11 & 1.944 & 0.983 & 0.125 & 0.444 & -0.444 & 0.768 & \\
\hline
\end{tabular}
\end{table}
C. NHBH

| i | j | I(i,j) | $\omega_{ij} \geq 0.1$ | $n = 2$, $s^z = 0$ |
|---|---|---|---|---|
| 1 | 8 | 2.609 | 0.981 | 0.443 | 0.542 | 0.642 | 0.466 |
| 7 | 12 | 2.595 | 0.986 | -0.372 | -0.534 | 0.534 | -0.539 |
| 2 | 3 | 2.480 | 0.971 | 0.602 | 0.503 | -0.503 | 0.364 |
| 5 | 9 | 1.909 | 0.889 | 0.227 | 0.517 | -0.517 | 0.644 |
| 6 | 10 | 1.909 | 0.889 | 0.227 | 0.517 | -0.517 | 0.644 |
| 5 | 10 | 0.197 | 0.235 | -0.079 | 0.481 | -0.481 | -0.729 |
| 6 | 9 | 0.197 | 0.235 | 0.079 | 0.481 | -0.481 | 0.729 |

| i | j | $I(i,j)$ | $\omega_{ij} \geq 0.1$ | $n = 3$, $s^z = -1/2$ | $n = 3$, $s^z = 1/2$ | $n = 4$ |
|---|---|---|---|---|---|---|
| 5 | 10 | 0.197 | 0.125 | 0.000 | 0.974 | 0.227 | 0.000 | 0.000 | 0.000 |
| 6 | 9 | 0.197 | 0.125 | 0.000 | -0.974 | 0.227 | 0.000 | 0.000 | 0.000 |

| i | j | $I(i,j)$ | $\omega_{ij} \geq 0.1$ | $n = 1$, $s^z = 1/2$ | $n = 1$, $s^z = -1/2$ |
|---|---|---|---|---|---|
| 5 | 10 | 0.197 | 0.125 | -0.974 | 0.227 | 0.000 | 0.000 |
| 6 | 9 | 0.197 | 0.125 | 0.974 | 0.227 | 0.000 | 0.000 | 0.000 |

| i | j | $I(i,j)$ | $\omega_{ij} \geq 0.1$ | $n = 1$, $s^z = -1/2$ |
|---|---|---|---|---|
| 5 | 10 | 0.197 | 0.125 | 0.000 | 0.000 | -0.974 | 0.227 |
| 6 | 9 | 0.197 | 0.125 | 0.000 | 0.000 | 0.974 | 0.227 |
D. CH$_3$CH$_3$

\[ n = 2, \ s^z = 0 \]
E. \text{CH}_2\text{CH}_2

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & \omega_{ij} > 0.1 & n = 2, \sigma^z = 0 \\
\hline
1 & 9 & 2.533 & 0.967 & -0.432 & -0.543 & 0.543 & -0.474 \\
2 & 10 & 2.533 & 0.967 & 0.432 & -0.543 & 0.543 & 0.474 \\
8 & 14 & 2.533 & 0.967 & 0.432 & -0.543 & 0.543 & 0.474 \\
7 & 13 & 2.533 & 0.967 & 0.432 & -0.543 & 0.543 & 0.474 \\
3 & 12 & 2.478 & 0.979 & 0.384 & -0.594 & 0.594 & 0.384 \\
5 & 11 & 2.414 & 0.937 & 0.475 & -0.523 & 0.523 & 0.475 \\
\hline
\end{tabular}
\end{table}
F. CHCH

\[ n = 2, \sigma^z = 0 \]

| i | j | I(i,j) | \( \omega_{ij} > 0.1 \) |
|---|---|---|---|
| 7 | 12 | 2.628 | 0.986 | -0.415 | -0.540 | 0.540 | 0.495 |
| 1 | 8 | 2.628 | 0.986 | -0.415 | -0.540 | 0.540 | -0.495 |
| 2 | 3 | 2.609 | 0.976 | -0.483 | -0.516 | 0.516 | -0.483 |
| 5 | 10 | 2.031 | 0.866 | 0.417 | -0.571 | 0.571 | 0.417 |
| 6 | 9 | 2.031 | 0.866 | -0.417 | -0.571 | 0.571 | -0.417 |
| 5 | 9 | 0.240 | 0.230 | 0.286 | -0.647 | 0.647 | 0.286 |
| 6 | 10 | 0.240 | 0.230 | 0.286 | -0.647 | 0.647 | 0.286 |
G. \textbf{SiH}_3\textbf{CH}_3

| i | j | I(i,j) | \(\alpha_{\omega} > 0.1\) |
|---|---|-------|------------------------|
| 11 | 20 | 2.583 | 0.977 | -0.431 | -0.543 | 0.543 | -0.435 |
| 12 | 13 | 2.583 | 0.977 | -0.435 | -0.543 | 0.543 | -0.471 |
| 10 | 19 | 2.583 | 0.977 | -0.471 | -0.543 | 0.543 | -0.435 |
| 3  | 7  | 2.442 | 0.950 | 0.378  | -0.542 | 0.542 | 0.520  |
| 4  | 14 | 2.442 | 0.950 | -0.378 | -0.542 | 0.542 | -0.520 |
| 5  | 15 | 2.442 | 0.950 | 0.378  | -0.542 | 0.542 | 0.520  |
| 17 | 18 | 2.284 | 0.924 | -0.553 | 0.533  | -0.533 | -0.356 |
H. SiH₂CH₂

| i  | j  | I(i,j) | ω_{ij} > 0.1 |
|----|----|--------|--------------|
| 12 | 18 | 2.586  | 0.977        |
| 8  | 9  | 2.586  | 0.977        |
| 1  | 2  | 2.404  | 0.942        |
| 4  | 6  | 2.404  | 0.942        |
| 7  | 17 | 2.371  | 0.934        |
| 11 | 15 | 2.301  | 0.958        |

| n = 2, s^z = 0 |
|----------------|
| - - ↑↓ ↑↓ ↑↓ - |

Orbital index

| i  | j  | I(i,j) | ω_{ij} > 0.1 |
|----|----|--------|--------------|
| 12 | 18 | 2.586  | 0.977        |
| 8  | 9  | 2.586  | 0.977        |
| 1  | 2  | 2.404  | 0.942        |
| 4  | 6  | 2.404  | 0.942        |
| 7  | 17 | 2.371  | 0.934        |
| 11 | 15 | 2.301  | 0.958        |
### I. SiHCH

| i | j | $I(i,j)$ | $\omega_{i,j}$ | $n = 2, s^z = 0$ |
|---|---|---|---|---|
| 1 | 12 | 2.586 | 0.977 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 10 | 11 | 2.349 | 0.921 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 5 | 6 | 2.279 | 0.912 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 3 | 15 | 2.108 | 0.898 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 2 | 14 | 2.108 | 0.898 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 2 | 15 | 0.122 | 0.203 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 3 | 14 | 0.122 | 0.203 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 7 | 14 | 0.114 | 0.213 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |
| 8 | 15 | 0.114 | 0.213 | $\uparrow \downarrow, \downarrow \uparrow, \uparrow \downarrow, \uparrow \downarrow$ |

| i | j | $I(i,j)$ | $\omega_{i,j}$ | $n = 0$ | $n = 3, s^z = -1/2$ | $n = 3, s^z = 1/2$ | $n = 4$ |
|---|---|---|---|---|---|---|---|
| 7 | 14 | 0.329 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 8 | 15 | 0.328 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |

---

**Orbital index**

- **$I(i,j)$**: Interaction between orbitals $i$ and $j$.
- **$\omega_{i,j}$**: Coupling constant.
- **$n = 2, s^z = 0$**: Spin states for $n = 2$ with $s^z = 0$.
- **$n = 0$**: Spin states for $n = 0$.
- **$n = 3, s^z = -1/2$**: Spin states for $n = 3$ with $s^z = -1/2$.
- **$n = 3, s^z = 1/2$**: Spin states for $n = 3$ with $s^z = 1/2$.
- **$n = 4$**: Spin states for $n = 4$.
III. DELOCALIZED SYSTEMS

A. CH$_2$CH$_2$BH$_2$

| $i$ | $j$ | $\omega_{ij}$ | $n = 2$, $s^z = 0$ |
|-----|-----|--------------|-----------------|
| 14  | 20  | 2.633        | -0.427 -0.541 0.541 -0.483 |
| 9   | 10  | 2.625        | 0.426 0.541 -0.541 0.483 |
| 1   | 12  | 2.538        | -0.432 -0.543 0.543 -0.474 |
| 13  | 14  | 2.532        | 0.476 -0.542 0.542 -0.430 |
| 7   | 17  | 2.459        | 0.435 -0.543 0.543 -0.471 |
| 8   | 17  | 2.459        | 0.397 0.529 -0.529 -0.532 |
| 4   | 5   | 2.396        | 0.466 0.524 -0.524 -0.484 |
| 16  | 19  | 0.434        | 0.063 -0.321 0.321 0.889 |
| 2   | 19  | 0.367        | -0.062 -0.437 0.437 -0.784 |

| $i$ | $j$ | $\omega_{ij}$ | $n = 3$, $s^z = -1/2$ | $n = 3$, $s^z = 1/2$ | $n = 4$ |
|-----|-----|--------------|-----------------|-----------------|--------|
| 16  | 19  | 0.434        | 1.000 0.000 0.000 0.000 | 0.000 0.000 0.000 0.000 |
| 2   | 19  | 0.367        | 1.000 0.000 0.000 0.000 | 0.000 0.000 0.000 0.000 |

| $i$ | $j$ | $\omega_{ij}$ | $n = 1$, $s^z = 1/2$ | $n = 1$, $s^z = -1/2$ |
|-----|-----|--------------|-----------------|-----------------|
| 16  | 19  | 0.434        | -0.947 0.321 0.000 0.000 | 0.947 -0.321 |
| 2   | 19  | 0.367        | 0.971 0.240 0.000 0.000 | 0.000 0.000 |

| $i$ | $j$ | $\omega_{ij}$ | $n = 1$, $s^z = 1/2$ | $n = 1$, $s^z = -1/2$ |
|-----|-----|--------------|-----------------|-----------------|
| 16  | 19  | 0.434        | -0.947 0.321 0.000 0.000 | 0.947 -0.321 |
## B. CH$_2$CH$_2$NH$_2$

| $i$ | $j$ | $I(i,j)$ | $\omega_{\alpha} > 0.1$ | $n = 2, s^z = 0$ |
|-----|-----|---------|----------------|----------------|
| 1   | 3   | 2.469   | 0.979          | -0.386 -0.537 0.537 -0.524 |
| 4   | 14  | 2.556   | 0.976          | 0.525 -0.537 0.537 0.386 |
| 11  | 19  | 2.531   | 0.966          | -0.439 -0.542 0.542 -0.469 |
| 12  | 20  | 2.523   | 0.964          | 0.436 -0.542 0.542 0.471 |
| 6   | 16  | 2.496   | 0.959          | -0.473 -0.543 0.543 -0.433 |
| 5   | 15  | 2.459   | 0.953          | 0.398 0.529 -0.529 0.531 |
| 8   | 18  | 2.414   | 0.937          | 0.488 0.523 -0.523 0.462 |
| 10  | 17  | 1.987   | 0.832          | 0.540 -0.589 0.589 0.436 |
| 2   | 17  | 0.526   | 0.221          | 0.079 0.358 -0.358 0.859 |
| 2   | 10  | 0.432   | 0.187          | 0.085 -0.482 0.482 -0.727 |

| $i$ | $j$ | $I(i,j)$ | $\omega_{\alpha} > 0.1$ | $n = 0$ | $n = 3, s^z = -1/2$ | $n = 3, s^z = 1/2$ | $n = 4$ |
|-----|-----|---------|----------------|------|----------------|----------------|------|
| 2   | 17  | 0.526   | 0.334          | 0.000 | 0.000 -0.334 0.334 | 0.000 | 0.000 -0.357 0.357 | 0.000 | 0.000 1.000 |
| 2   | 10  | 0.432   | 0.319          | 0.000 | 0.000 -0.357 0.357 | 0.000 | 0.000 -0.957 0.957 | 0.000 | 0.000 1.000 |

### Diagrams

[Diagram of orbital index and energy levels for CH$_2$CH$_2$NH$_2$.]
C. Butadiene

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & \omega_\alpha > 0.1 & n = 2, s^z = 0 \\
\hline
1 & 16 & 2.533 & 0.967 & -0.542 & 0.542 & 0.474 \\
15 & 26 & 2.532 & 0.967 & -0.542 & 0.542 & 0.474 \\
2 & 17 & 2.529 & 0.966 & -0.542 & 0.542 & 0.474 \\
14 & 25 & 2.529 & 0.966 & -0.542 & 0.542 & 0.474 \\
7 & 20 & 2.492 & 0.958 & 0.433 & 0.542 & 0.474 \\
9 & 22 & 2.492 & 0.958 & 0.433 & 0.542 & 0.474 \\
4 & 5 & 2.406 & 0.935 & 0.474 & 0.524 & 0.474 \\
10 & 11 & 2.406 & 0.935 & 0.474 & 0.524 & 0.474 \\
8 & 21 & 2.482 & 0.934 & 0.433 & 0.536 & 0.474 \\
13 & 23 & 2.129 & 0.908 & 0.380 & 0.594 & 0.388 \\
3 & 13 & 0.120 & 0.217 & 0.221 & 0.672 & 0.672 & 0.221 \\
\hline
\end{array}
\]
D. Cyclopentadiene

| i | j | I(i,j) | $\omega_{ij} > 0.1$ | $n = 2, s^z = 0$ |
|---|---|-------|-----------------|-----------------|
| 1 | 2 | 2.347 | 0.970 | -0.542 | 0.542 | 0.433 |
| 15 | 20 | 2.345 | 0.969 | -0.542 | 0.542 | 0.475 |
| 1 | 19 | 2.342 | 0.969 | -0.542 | 0.542 | 0.475 |
| 18 | 31 | 2.341 | 0.968 | -0.542 | 0.542 | 0.433 |
| 9 | 10 | 2.486 | 0.957 | 0.543 | 0.543 | 0.475 |
| 25 | 26 | 2.481 | 0.956 | -0.543 | 0.543 | 0.475 |
| 4 | 7 | 2.328 | 0.921 | 0.540 | -0.540 | 0.454 |
| 11 | 28 | 2.327 | 0.921 | 0.540 | -0.540 | 0.459 |
| 3 | 5 | 2.302 | 0.910 | 0.524 | 0.524 | 0.475 |
| 14 | 16 | 2.299 | 0.909 | 0.524 | 0.524 | 0.475 |
| 12 | 24 | 2.236 | 0.897 | 0.537 | 0.537 | 0.460 |
| 17 | 27 | 2.024 | 0.879 | 0.592 | 0.592 | 0.385 |
| 23 | 27 | 2.023 | 0.879 | 0.592 | 0.592 | 0.385 |
| 25 | 27 | 0.173 | 0.219 | 0.620 | 0.620 | 0.340 |
| 2 | 17 | 0.119 | 0.208 | 0.664 | 0.664 | -0.244 |
E. Hexatriene

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 21| 37| 2.584| 0.976| 0.433| -0.544| 0.543| 0.473|
| 22| 38| 2.584| 0.976| 0.433| -0.544| 0.544| 0.473|
| 1 | 23| 2.556| 0.971| 0.433| -0.543| 0.541| 0.475|
| 16| 33| 2.554| 0.971| -0.469| -0.542| 0.543| -0.437|
| 2 | 24| 2.547| 0.969| -0.431| -0.543| 0.541| -0.476|
| 9 | 28| 2.522| 0.964| -0.433| -0.542| 0.543| -0.474|
| 10| 32| 2.508| 0.962| -0.433| -0.544| 0.540| -0.473|
| 15| 34| 2.508| 0.962| -0.435| -0.541| 0.544| -0.471|
| 18| 19| 2.465| 0.947| -0.470| 0.525| -0.522| -0.481|
| 17| 31| 2.455| 0.947| -0.463| 0.538| -0.534| -0.499|
| 10| 27| 2.435| 0.945| 0.460| 0.538| -0.534| 0.462|
| 4 | 5 | 2.431| 0.940| 0.474| 0.525| -0.523| 0.476|
| 11| 12| 2.421| 0.938| 0.471| 0.527| -0.521| -0.478|
| 6 | 25| 2.133| 0.910| -0.384| 0.586| -0.604| -0.381|
| 34| 36| 2.107| 0.904| -0.390| 0.608| -0.584| -0.369|
| 14| 30| 1.770| 0.831| 0.348| 0.575| -0.634| -0.382|
| 14| 34| 0.191| 0.243| 0.321| 0.539| -0.706| 0.328|
| 6 | 30| 0.173| 0.233| -0.314| -0.537| 0.713| -0.324|
| 30| 36| 0.117| 0.228| 0.222| -0.766| 0.576| 0.177|
| 14| 25| 0.103| 0.216| 0.189| -0.311| 0.711| 0.269|

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 14| 34| 0.191| 0.106| 0.000| 1.000|
| 6 | 30| 0.173| 0.109| 1.000| 0.000|
| 30| 36| 0.117| 0.102| 1.000| 0.000|
| 14| 25| 0.103| 0.105| 0.000| 1.000|

\( n = 2, s^z = 0 \)

\( \rho(n, s^z) = 0 \)

\( \omega_{n, s^z} > 0.1 \)

\( \alpha \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \beta \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \gamma \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \delta \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \epsilon \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \zeta \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \eta \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \theta \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \iota \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \kappa \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \lambda \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \mu \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \nu \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \xi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \psi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \chi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \psi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \chi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \phi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \psi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \chi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \phi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \psi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \chi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \phi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)

\( \psi \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \)
IV. ANTIROMATICITY

A. Cyclobutadiene

| i  | j  | ω_{ij} | n = 2, s^z = 0 |
|----|----|--------|----------------|
| 13 | 23 | 0.544  | 0.431, 0.541, 0.541, 0.478 |
| 14 | 24 | 0.544  | 0.431, 0.541, 0.541, 0.478 |
| 16 | 17 | 0.544  | 0.478, -0.541, 0.541, 0.431 |
| 15 | 25 | 0.544  | 0.431, -0.541, 0.541, 0.478 |
| 12 | 22 | 0.544  | 0.376, -0.549, 0.599, -0.376 |
| 2 | 18 | 2.544  | 0.969, 0.376, -0.549, 0.599, -0.376 |
| 9 | 10 | 2.544  | 0.969, 0.475, -0.524, 0.524, 0.475 |
| 5 | 6 | 2.544  | 0.969, 0.475, -0.524, 0.524, 0.475 |
| 8 | 19 | 0.544  | 0.445, 0.550, -0.550, 0.445 |
| 7 | 20 | 1.973  | 0.355, 0.590, -0.590, 0.422 |
| 5 | 19 | 0.118  | 0.157, 0.355, 0.590, -0.590, 0.422 |
| 10 | 20 | 0.118  | 0.157, 0.355, 0.590, -0.590, 0.422 |
| 6 | 7 | 0.118  | 0.156, 0.355, 0.590, -0.590, 0.422 |
| 8 | 9 | 0.118  | 0.156, 0.422, 0.590, -0.590, -0.355 |
| 7 | 9 | 0.116  | 0.155, 0.423, 0.588, -0.588, 0.360 |
| 6 | 8 | 0.116  | 0.155, 0.360, -0.588, 0.588, 0.423 |
| 5 | 20 | 0.116  | 0.155, 0.360, -0.588, 0.588, 0.423 |
| 10 | 19 | 0.116  | 0.154, 0.359, 0.588, -0.588, -0.423 |
B. Borole

\begin{tabular}{|c|c|c|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & \(\omega_{\alpha} > 0.1\) & \(n = 2, \ s^z = 0\) & \(n = 2, \ s^z = -1/2\) & \(n = 3, \ s^z = -1/2\) & \(n = 3, \ s^z = 1/2\) & \(n = 4\) \\
\hline
17 & 29 & 2.610 & 0.980 & 0.429 & -0.540 & 0.540 & 0.482 & 0.482 \\
16 & 30 & 2.542 & 0.968 & 0.436 & -0.542 & 0.542 & 0.472 & 0.472 \\
9  & 23  & 2.540 & 0.968 & -0.433 & -0.542 & 0.542 & -0.474 & -0.474 \\
4  & 19  & 2.539 & 0.968 & 0.474 & -0.542 & 0.542 & 0.433 & 0.433 \\
5  & 18  & 2.536 & 0.967 & 0.436 & -0.542 & 0.542 & 0.472 & 0.472 \\
15 & 28  & 2.315 & 0.922 & -0.532 & 0.532 & -0.528 & -0.528 & -0.528 \\
8  & 11  & 2.285 & 0.966 & 0.466 & 0.524 & 0.524 & 0.484 & 0.484 \\
10 & 12  & 2.282 & 0.905 & -0.542 & 0.542 & 0.472 & 0.472 & 0.472 \\
4  & 22  & 2.244 & 0.901 & 0.456 & 0.540 & -0.540 & 0.456 & 0.456 \\
20 & 21  & 2.058 & 0.882 & 0.502 & 0.595 & 0.595 & 0.562 & 0.562 \\
14 & 24  & 2.044 & 0.878 & 0.363 & 0.591 & 0.591 & 0.403 & 0.403 \\
24 & 27  & 0.215 & 0.119 & -0.635 & 0.397 & 0.397 & -0.826 & -0.826 \\
20 & 27  & 0.210 & 0.177 & -0.652 & 0.395 & 0.395 & -0.827 & -0.827 \\
14 & 27  & 0.189 & 0.162 & -0.637 & 0.253 & 0.253 & -0.933 & -0.933 \\
21 & 27  & 0.183 & 0.160 & -0.636 & 0.250 & 0.250 & -0.935 & -0.935 \\
\hline
\end{tabular}

\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & \(\omega_{\alpha} > 0.1\) & \(n = 0\) & \(n = 3, \ s^z = -1/2\) & \(n = 3, \ s^z = 1/2\) & \(n = 4\) \\
\hline
24 & 27 & 0.215 & 0.149 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 \\
20 & 27 & 0.210 & 0.148 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 \\
14 & 27 & 0.189 & 0.117 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 \\
21 & 27 & 0.183 & 0.116 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 \\
\hline
\end{tabular}

\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
i & j & I(i,j) & \(\omega_{\alpha} > 0.1\) & \(n = 1, \ s^z = 1/2\) & \(n = 1, \ s^z = -1/2\) \\
\hline
24 & 27 & 0.215 & 0.306 & 0.980 & 0.199 & 0.000 & 0.000 \\
20 & 27 & 0.210 & 0.306 & 0.981 & 0.196 & 0.000 & 0.000 \\
14 & 27 & 0.189 & 0.320 & -0.968 & 0.249 & 0.000 & 0.000 \\
21 & 27 & 0.183 & 0.320 & -0.969 & 0.246 & 0.000 & 0.000 \\
\hline
\end{tabular}
V. AROMATICITY

A. Benzene

| i   | j   | I(i,j) | \(\omega_{ij} > 0.1\) |
|-----|-----|--------|----------------------|
| 16  | 33  | 2.556  | 0.971                |
| 3   | 8   | 2.553  | 0.970                |
| 7   | 24  | 2.551  | 0.970                |
| 17  | 31  | 2.550  | 0.970                |
| 1   | 22  | 2.544  | 0.969                |
| 21  | 36  | 2.540  | 0.968                |
| 12  | 29  | 2.522  | 0.961                |
| 10  | 11  | 2.521  | 0.961                |
| 19  | 32  | 2.519  | 0.960                |
| 4   | 5   | 2.517  | 0.960                |
| 6   | 25  | 2.517  | 0.960                |
| 2   | 26  | 0.899  | 0.524                |
| 30  | 35  | 0.898  | 0.523                |
| 15  | 35  | 0.891  | 0.521                |
| 2   | 9   | 0.889  | 0.520                |
| 15  | 26  | 0.886  | 0.519                |
| 9   | 15  | 0.885  | 0.519                |
| 26  | 30  | 0.882  | 0.519                |
| 2   | 35  | 0.877  | 0.529                |

\(n = 2, s^z = 0\)
B. Pyrrole

\[ I(i,j) = 2, \quad s_z = 0 \]

\[ \omega_\alpha > 0.1 \quad , \quad \omega_\alpha > 0.1 \]

\[ n = 2, \quad s_z = 0 \quad n = 3, \quad s_z = 1/2 \]

\[ n = 3, \quad s_z = 1/2 \quad n = 4 \]

| i | j | I(i,j) | \omega_\alpha > 0.1 | n = 0 | n = 3, s_z = -1/2 | n = 3, s_z = 1/2 | n = 4 |
|---|---|-------|------------------|------|-----------------|-----------------|------|
| 14 | 30 | 2.582 | 0.976 | -0.436 | -0.541 | 0.541 | 0.473 |
| 3 | 20 | 2.376 | 0.975 | -0.435 | -0.541 | 0.541 | 0.474 |
| 1 | 19 | 2.573 | 0.974 | -0.431 | -0.541 | 0.541 | 0.478 |
| 18 | 29 | 2.570 | 0.974 | -0.479 | -0.541 | 0.541 | 0.430 |
| 10 | 25 | 2.542 | 0.976 | -0.375 | -0.535 | 0.535 | -0.535 |
| 15 | 27 | 2.378 | 0.928 | -0.461 | 0.525 | -0.525 | -0.486 |
| 4 | 23 | 2.374 | 0.928 | 0.486 | 0.525 | -0.525 | 0.461 |
| 2 | 7 | 2.358 | 0.938 | -0.555 | 0.524 | -0.524 | -0.378 |
| 11 | 28 | 2.348 | 0.936 | 0.377 | 0.524 | -0.524 | 0.556 |
| 12 | 24 | 2.344 | 0.922 | 0.466 | 0.532 | -0.532 | 0.465 |
| 17 | 20 | 1.385 | 0.652 | 0.396 | 0.586 | -0.586 | -0.395 |
| 5 | 21 | 1.384 | 0.651 | 0.394 | 0.587 | -0.587 | 0.396 |
| 9 | 21 | 0.585 | 0.264 | 0.209 | 0.521 | -0.521 | -0.643 |
| 17 | 10 | 0.582 | 0.263 | 0.209 | 0.521 | -0.521 | -0.643 |
| 5 | 26 | 0.515 | 0.351 | 0.391 | -0.589 | 0.589 | 0.392 |
| 5 | 9 | 0.166 | 0.151 | 0.721 | 0.484 | -0.484 | 0.109 |
| 9 | 26 | 0.165 | 0.150 | 0.108 | 0.383 | -0.383 | -0.723 |
| 17 | 21 | 0.164 | 0.199 | 0.301 | -0.639 | 0.639 | 0.303 |
### C. Furan

\[
\begin{align*}
I(i,j) & \omega_\alpha > 0.1 & n = 0 & n = 3, s^z = -1/2 & n = 3, s^z = 1/2 & n = 4 \\
\hline
1 & 26 & 2.559 & 0.972 & -0.431 & -0.541 & 0.541 & -0.480 \\
1 & 19 & 2.552 & 0.971 & -0.429 & -0.541 & 0.541 & -0.480 \\
2 & 20 & 2.548 & 0.970 & -0.425 & -0.541 & 0.541 & -0.484 \\
17 & 18 & 2.539 & 0.968 & -0.426 & -0.541 & 0.541 & 0.483 \\
15 & 27 & 2.322 & 0.914 & -0.485 & 0.525 & -0.525 & 0.463 \\
4 & 5 & 2.322 & 0.915 & -0.486 & 0.524 & -0.524 & 0.463 \\
6 & 24 & 2.251 & 0.899 & -0.463 & 0.553 & -0.553 & 0.465 \\
7 & 8 & 2.074 & 0.817 & 0.588 & -0.319 & 0.319 & 0.339 \\
14 & 28 & 2.068 & 0.875 & 0.340 & 0.519 & -0.519 & 0.587 \\
4 & 22 & 1.493 & 0.691 & 0.399 & 0.587 & -0.587 & 0.391 \\
25 & 29 & 1.488 & 0.690 & 0.399 & -0.587 & 0.587 & 0.391 \\
9 & 29 & 0.521 & 0.241 & 0.179 & 0.502 & -0.502 & 0.680 \\
9 & 22 & 0.514 & 0.239 & 0.178 & 0.502 & -0.502 & 0.681 \\
3 & 25 & 0.431 & 0.320 & 0.389 & -0.591 & 0.591 & 0.388 \\
9 & 25 & 0.170 & 0.158 & 0.092 & 0.502 & -0.502 & 0.757 \\
3 & 9 & 0.168 & 0.158 & 0.768 & 0.357 & -0.457 & 0.091 \\
12 & 28 & 0.160 & 0.331 & 0.006 & -0.232 & 0.232 & 0.945 \\
7 & 12 & 0.159 & 0.331 & -0.945 & 0.231 & -0.231 & -0.006 \\
22 & 29 & 0.143 & 0.193 & 0.290 & -0.644 & 0.644 & 0.293 \\
8 & 12 & 0.132 & 0.121 & -0.939 & 0.243 & -0.243 & -0.006 \\
12 & 14 & 0.132 & 0.121 & -0.006 & 0.242 & -0.242 & -0.939
\end{align*}
\]
D. Thiophene

\[
I(i,j) = \frac{1}{2} \omega_{\alpha} > 0.1 \qquad \begin{array}{c|c|c|c|c}
\omega_{\alpha} & n = 2, s^z = 0 & n = 3, s^z = -\frac{1}{2} & n = 3, s^z = \frac{1}{2} & n = 4
\hline
22 & 35 & 2.560 & 0.970 & 0.430 & -0.541 & 0.541 & 0.479
23 & 28 & 2.547 & 0.969 & 0.434 & -0.542 & 0.542 & 0.474
21 & 2 & 2.542 & 0.969 & 0.480 & 0.541 & -0.541 & 0.429
18 & 32 & 2.536 & 0.967 & 0.432 & -0.542 & 0.542 & 0.476
30 & 31 & 2.374 & 0.926 & 0.485 & 0.524 & -0.524 & 0.464
35 & 5 & 2.369 & 0.925 & 0.461 & 0.524 & -0.524 & 0.482
16 & 27 & 2.341 & 0.922 & 0.463 & 0.534 & -0.534 & 0.464
19 & 28 & 2.126 & 0.864 & -0.471 & -0.538 & 0.538 & -0.446
8 & 26 & 2.125 & 0.863 & 0.447 & 0.538 & -0.538 & 0.470
6 & 24 & 1.642 & 0.750 & 0.396 & 0.589 & -0.589 & 0.387
21 & 29 & 1.640 & 0.749 & 0.388 & 0.589 & -0.589 & 0.395
13 & 24 & 0.413 & 0.208 & 0.134 & 0.446 & -0.445 & 0.765
13 & 22 & 0.412 & 0.208 & 0.434 & 0.446 & -0.445 & 0.566
6 & 29 & 0.451 & 0.292 & -0.380 & -0.597 & 0.597 & -0.379
8 & 14 & 0.182 & 0.199 & 0.944 & 0.234 & -0.234 & 0.911
14 & 26 & 0.177 & 0.234 & 0.010 & -0.292 & 0.292 & 0.911
14 & 19 & 0.176 & 0.235 & 0.010 & -0.290 & 0.290 & 0.912
6 & 13 & 0.155 & 0.161 & -0.846 & 0.374 & 0.375 & -0.846
13 & 29 & 0.155 & 0.160 & -0.060 & 0.375 & -0.375 & -0.060
21 & 24 & 0.142 & 0.205 & 0.277 & -0.651 & 0.651 & 0.275
21 & 24 & 0.142 & 0.205 & 0.277 & -0.651 & 0.651 & 0.275
\end{array}
\]