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Resolving the π-assisted U–N σ_f-bond formation using quantum information theory

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Supplementary Information

S1 Orbital-pair correlation diagrams

S1.1 UO_2^{2+}

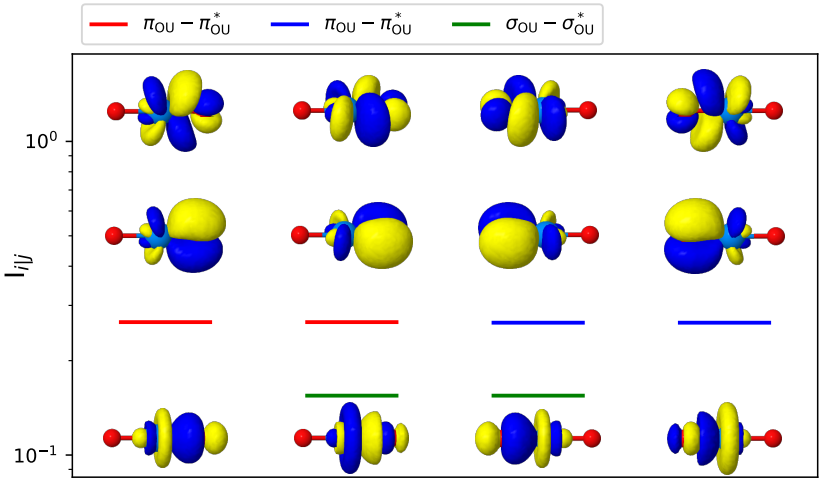

Figure S1: Selected orbital-pair correlation measures for the linear UO_2^{2+} molecule obtained from a fpLCCD wave function.

S1.2 NUO^+

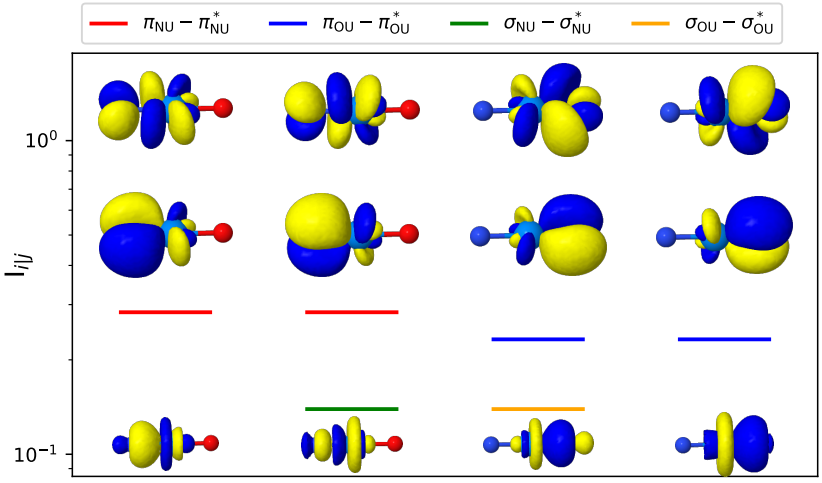

Figure S2: Selected orbital-pair correlation measures for the linear NUO^+ molecule obtained from a fpLCCD wave function.

S1.3 Reaction pathway

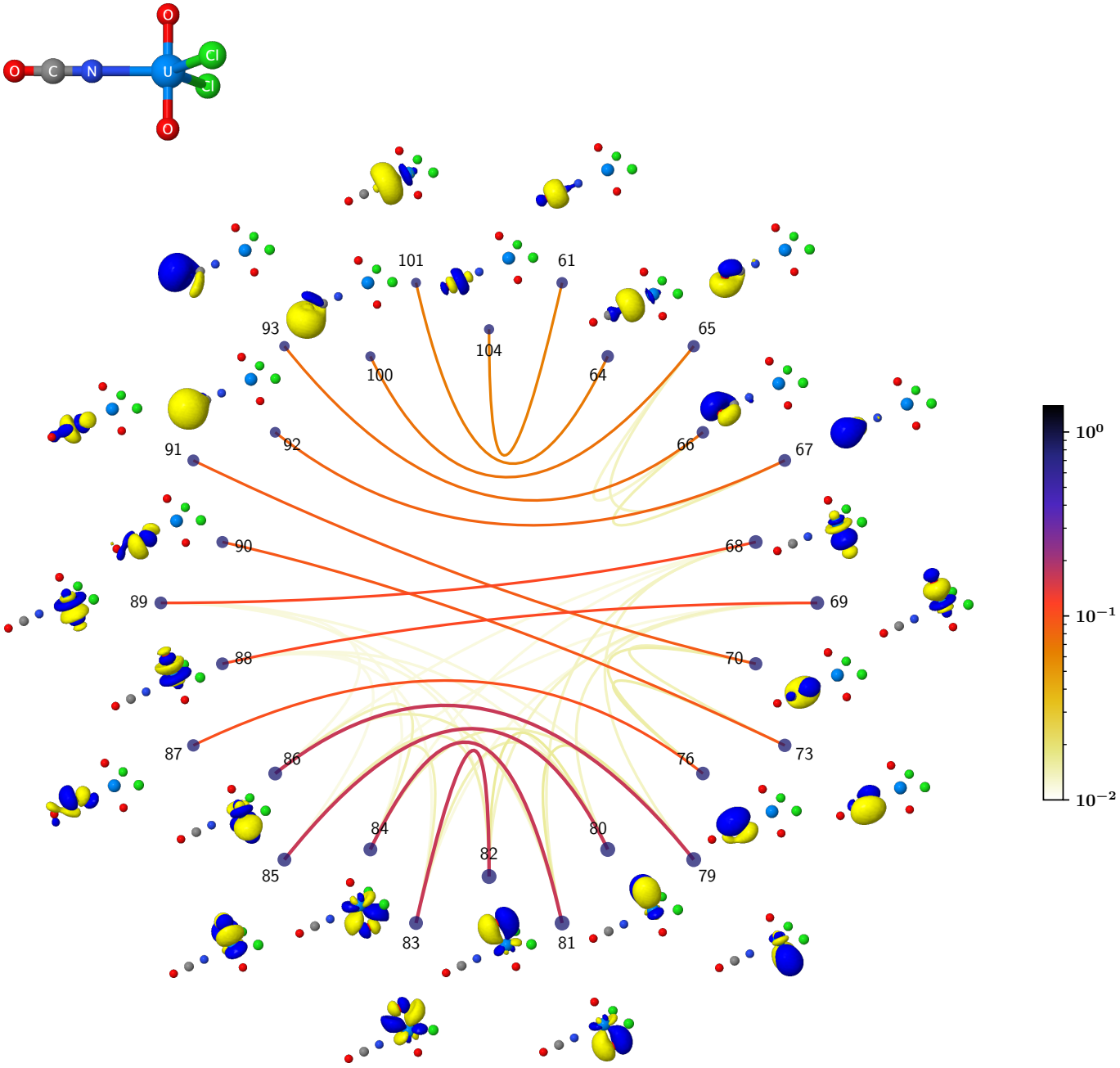

Figure S3: Orbital-pair correlation measures for the ground state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals.

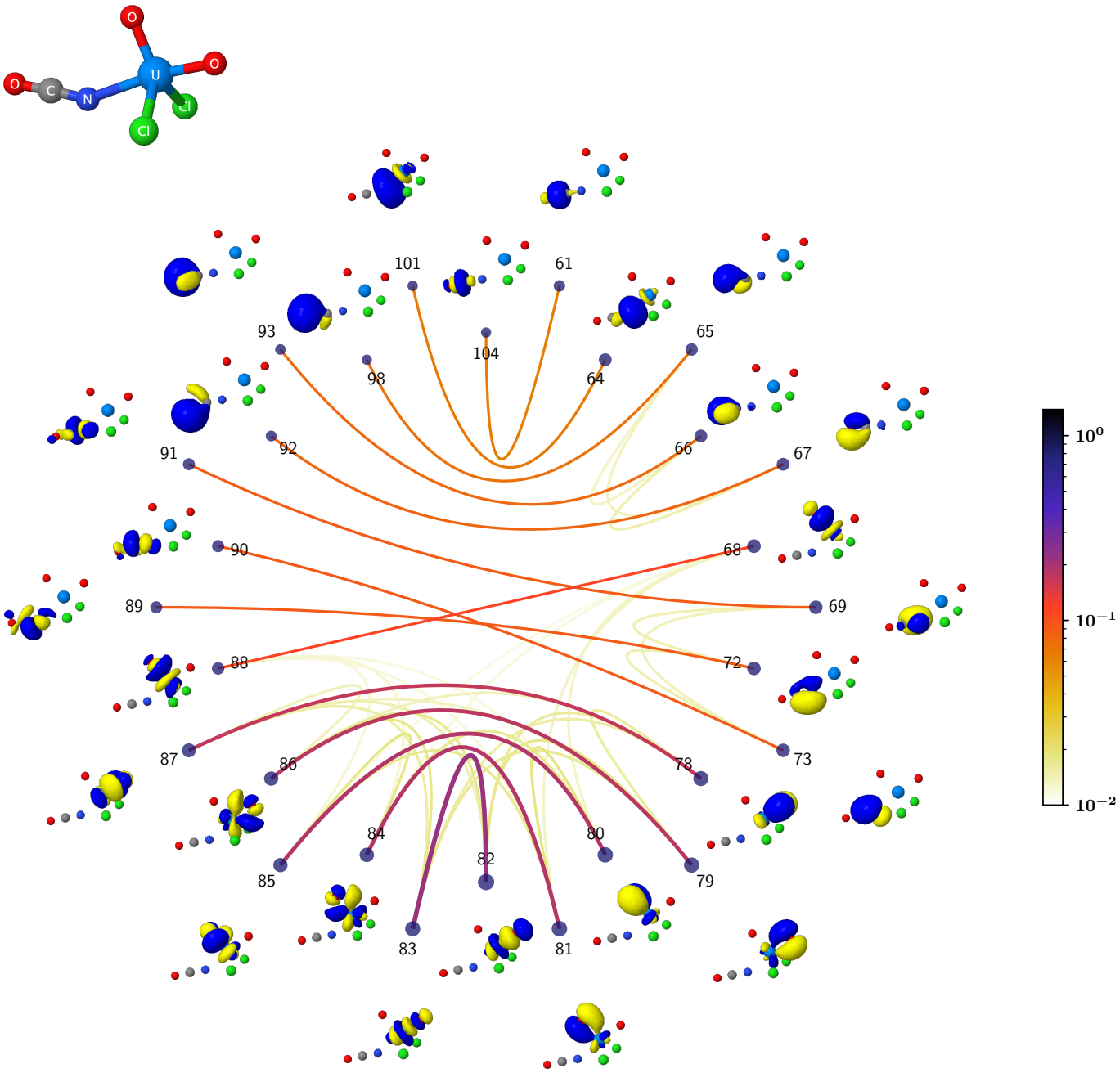

Figure S4: Orbital-pair correlation measures for the isomer of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

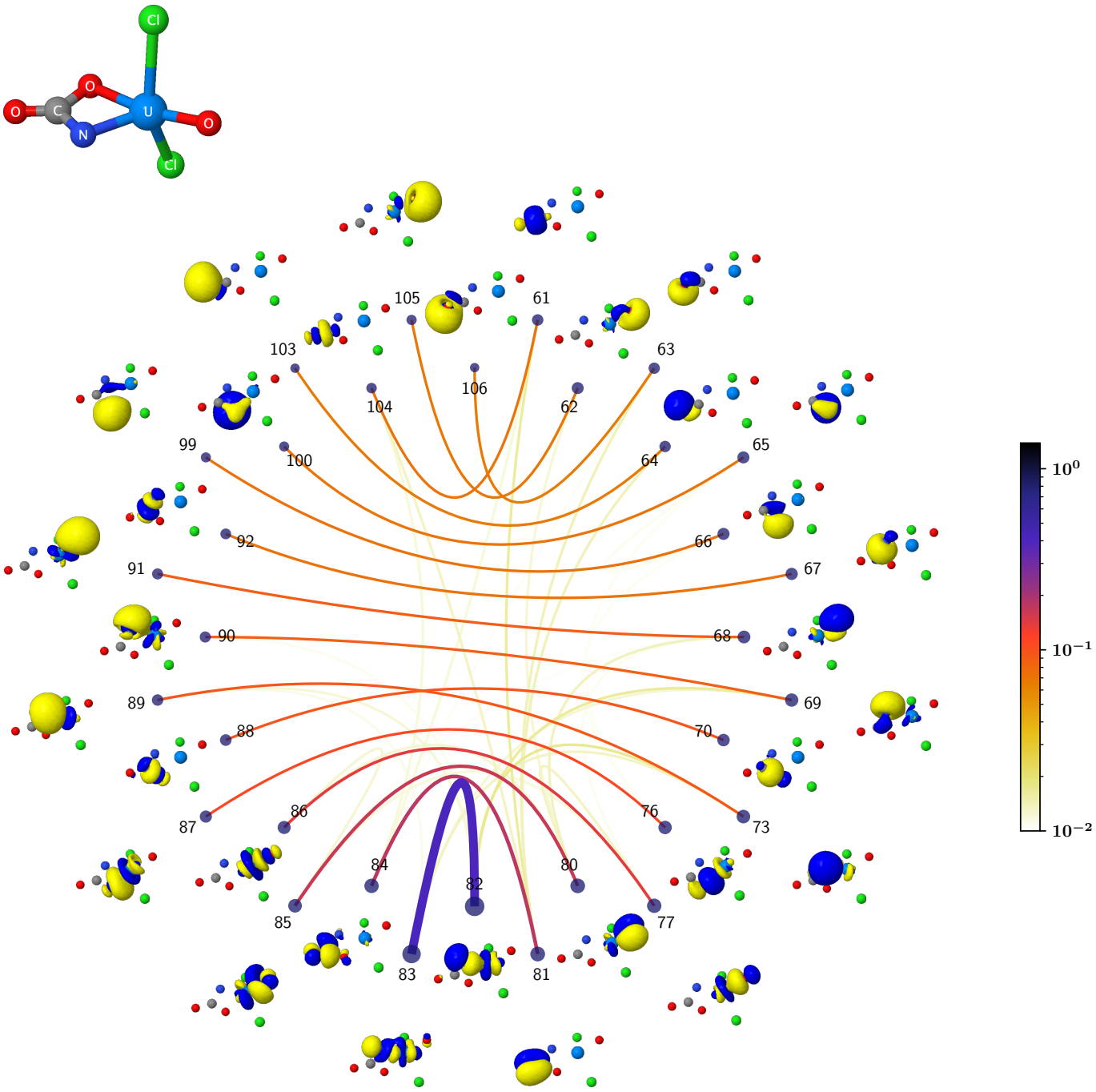

Figure S5: Orbital-pair correlation measures for the first transition state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

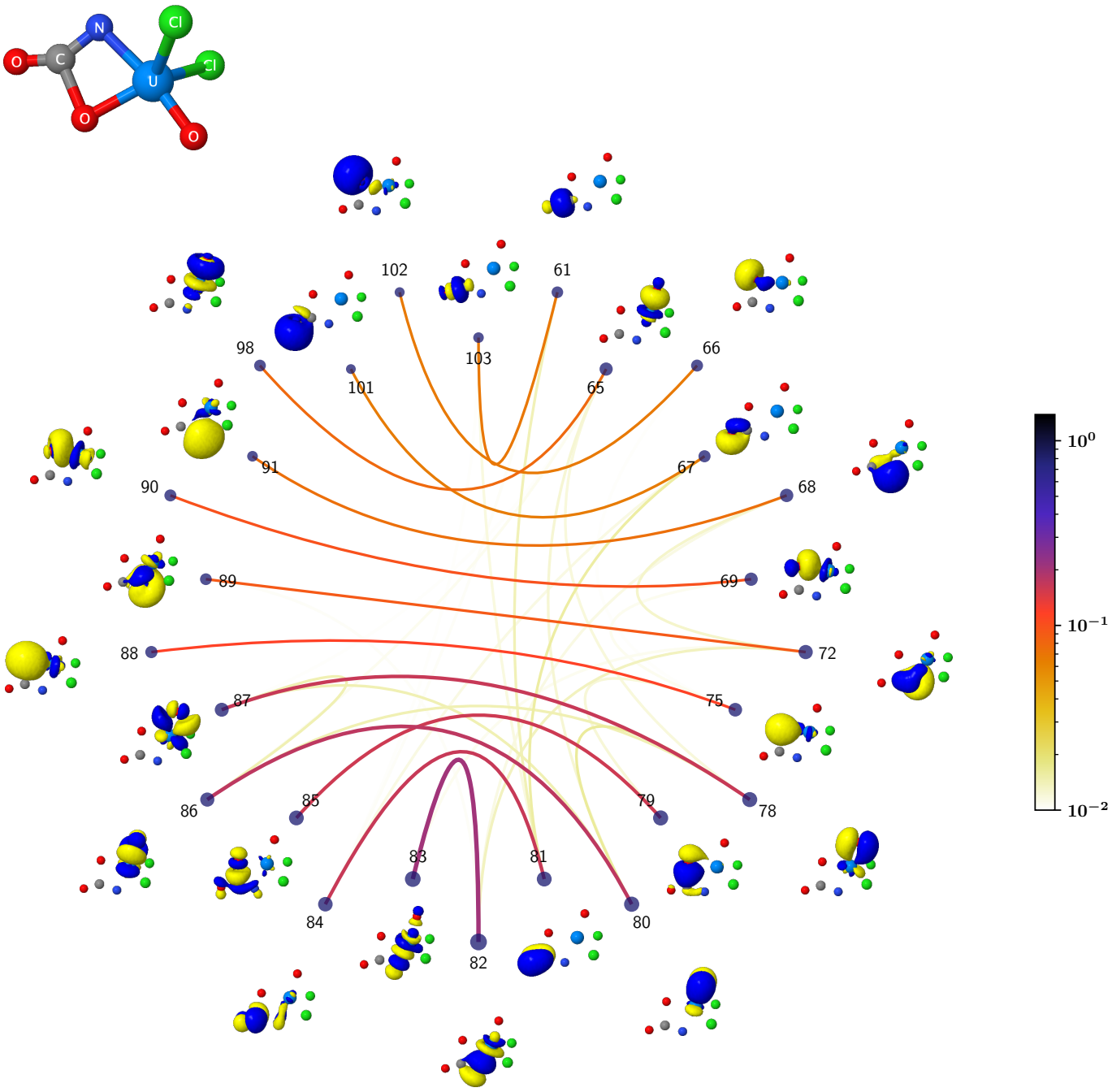

Figure S6: Orbital-pair correlation measures for the second transition state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

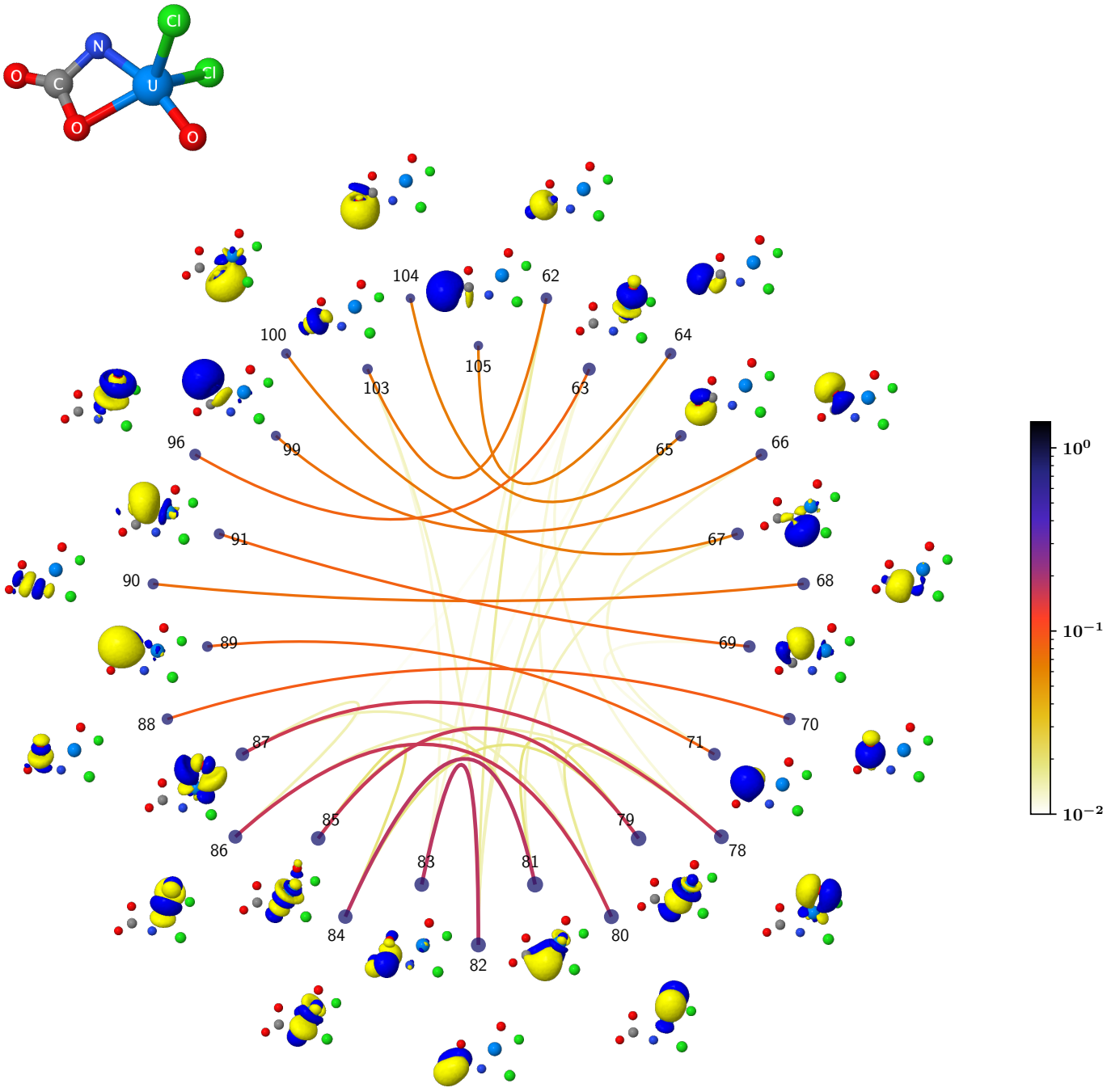

Figure S7: Orbital-pair correlation measures for the first intermediate state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

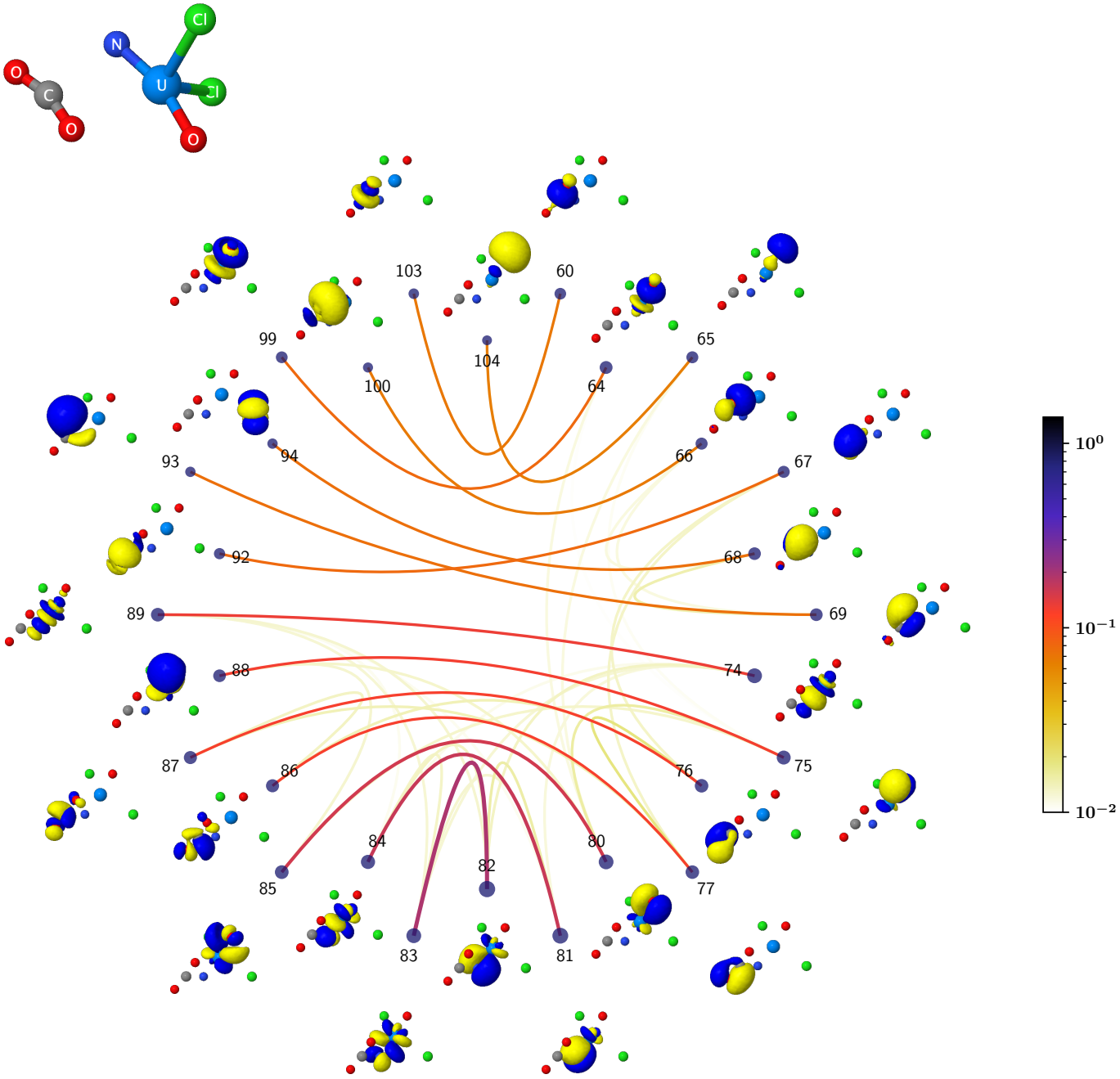

Figure S8: Orbital-pair correlation measures for the third transition state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

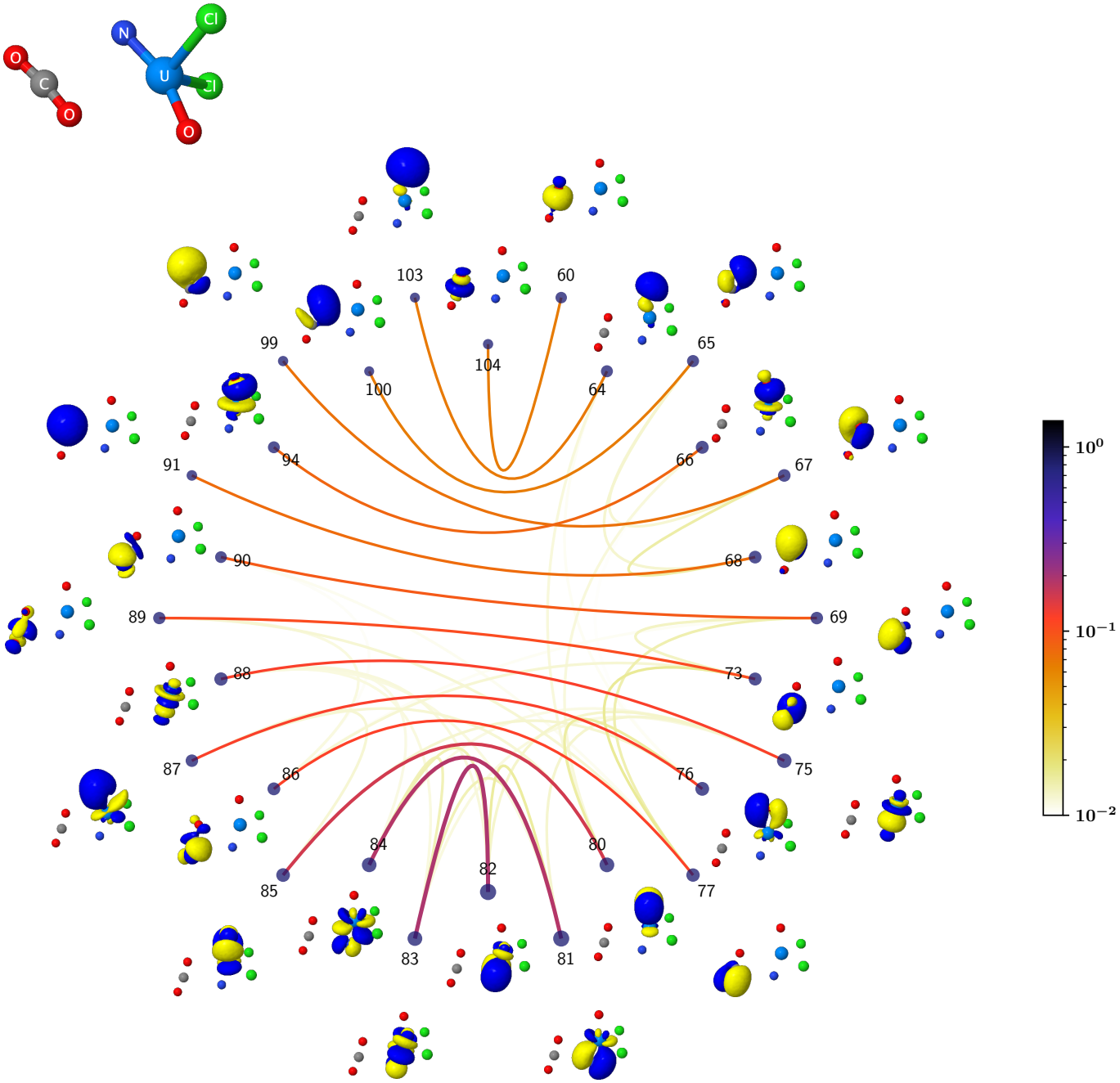

Figure S9: Orbital-pair correlation measures for the second intermediate state of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.

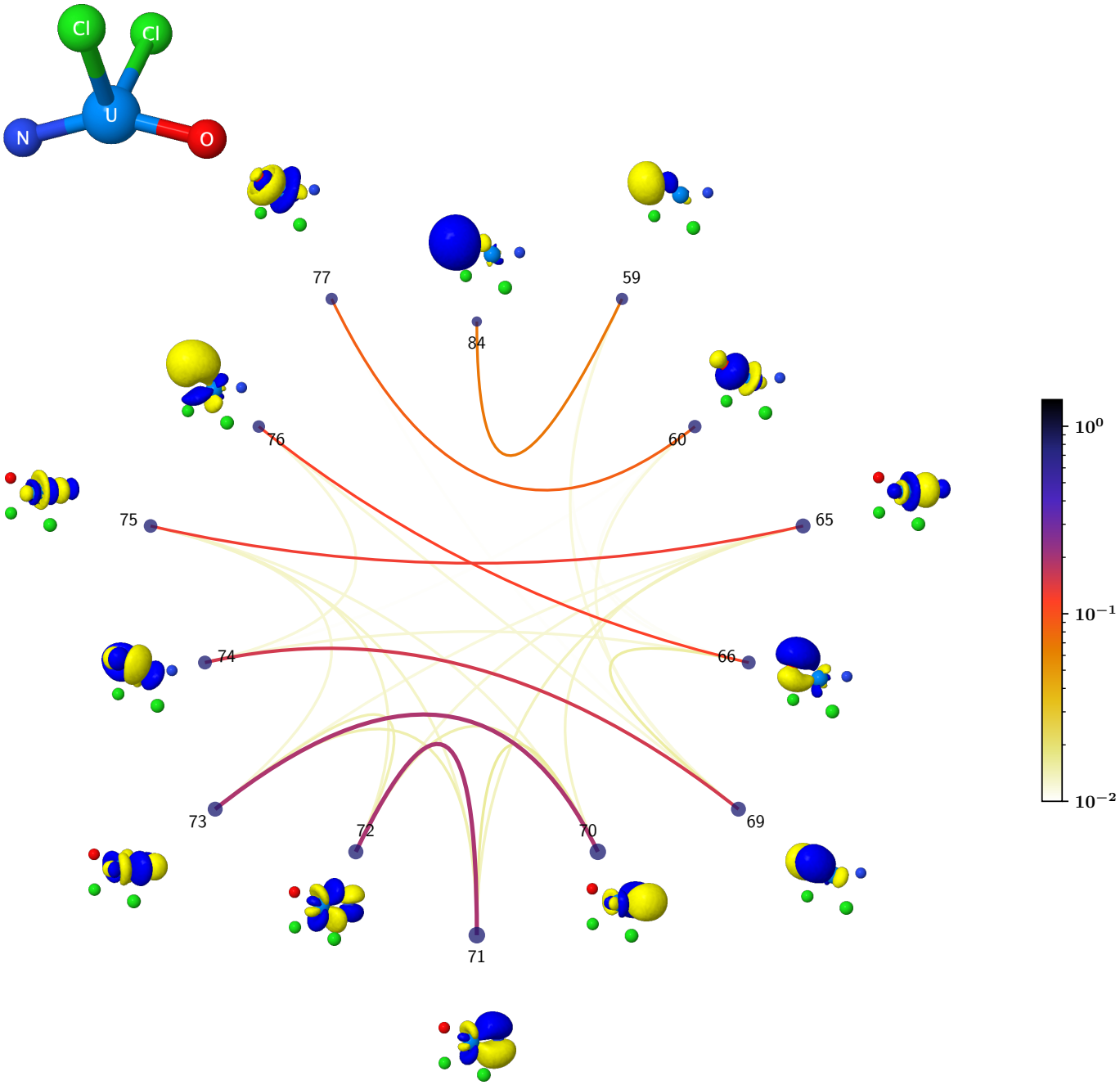

Figure S10: Orbital-pair correlation measures for $NUOCl_2$ of the reaction coordinate obtained from a fpLCCD wave function. The values of the single-orbital entropies are coded by the size of the dots corresponding to each orbital. The mutual information values correspond to color and width of lines connecting orbitals. All orbital-pair correlations larger than 0.09 have been plotted.