**Supplementary data**

**A quantum assessment of the interaction between Si12C12, BSi11C12, BSi12C11, NSi11C12 and NSi12C11 nanocages with Glycine amino acid: A DFT, TD-DFT and AIM study**

**M. Rezaei-Sameti\*1, M. Barandisheh Naghibi**

1\*Department of Applied Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran

**Figure S1** The bond length and bond angle Si12C12 nanocage before and after Al and N doped

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Model IV | Model III | Model II | Model I | Pristine |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |

**Figure S2** The bond length and bond angle Si12C12 nanocage and distance between Glycine and nanocage at A-a to F-c models.

|  |  |  |  |
| --- | --- | --- | --- |
| Distance between nanocluster and glycine | Angle bond | Length bond |  |
|  |  |  | MODEL A-a |
|  |  |  | MODEL A-b |
|  |  |  | MODEL A-c |
|  |  |  | MODEL B-a |
|  |  |  | MODEL B-b |
|  |  |  | MODEB B-c |
|  |  |  | MODEL C-a |
|  |  |  | MODEL C-b |
|  |  |  | MODEL C-c |
|  |  |  | MODEL D-a |
|  |  |  | MODEL D-b |
|  |  |  | MODEL D-c |
|  |  |  | MODELE-a |
|  |  |  | MODELE-b |
|  |  |  | MODELE-c |
|  |  |  | MODEL F-a |
|  |  |  | MODELF-b |
|  |  |  | MODELF-c |

**Table S1** The thermodynamic parameters of solvent (water) effect for A-a to F-a models

|  |  |  |
| --- | --- | --- |
| ∆∆G(sol)water kcal/mol | ∆G kcal/mol | Model |
| +3.93 | -24.20 | A-a |
| +0.34 | -27.61 | B-a |
| +13.02 | -20.23 | C-a |
| +10.06 | -23.22 | D-a |
| +4.96 | -27.60 | E-a |
| +4.07 | -30.01 | F-a |

**Table S2** Quantum parameters for adsorption of glycine on the surface of pristine and N,B doped C12Si12 for A-a to F-c models

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pristine | MODEL B-c | MODEL B-b | MODEL B-a | property |
| -6.03 | -5.69 | -5.34 | -5.36 | E HOMO(ev) |
| -2.80 | -2.44 | -2.14 | -2.20 | E LUMO(ev) |
| +3.23 | +3.25 | +3.20 | +3.16 | E gap |
| -4.42 | -4.07 | -3.74 | -3.78 | E Fermi |
| +2.80 | +2.44 | +2.14 | +2.20 | A |
| +6.03 | +5.69 | +5.34 | +5.36 | I |
| +1.61 | +1.62 | +1.60 | +1.58 | η |
| +0.30 | +0.30 | +0.31 | +0.31 | S |
| -4.42 | -4.07 | -3.74 | -3.78 | µ |
| -1.61 | -1.62 | -1.6 | -1.58 | ∆ф |
| +2.73 | +2.50 | +2.33 | +2.38 | ∆N |
| +9.77 | +5.09 | +4.37 | +4.51 | ω |
| +4.42 | +4.07 | +3.74 | +3.78 | X |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ristine | MODEL B-c | MODEL B-b | MODEL B-a | property |
| -6.03 | -5.83 | -5.33 | -5.13 | E HOMO(ev) |
| -2.80 | -2.61 | -2.12 | -2.15 | E LUMO(ev) |
| +3.23 | +3.22 | +3.20 | +2.97 | E gap |
| -4.42 | -4.22 | -3.72 | -3.64 | E Fermi |
| +2.80 | +2.61 | +2.12 | +2.15 | A |
| +6.03 | +5.83 | +5.33 | +5.13 | I |
| +1.61 | +1.61 | +1.60 | +1.49 | η |
| +0.30 | +0.31 | +0.31 | +0.33 | S |
| -4.42 | -4.22 | -3.72 | -3.64 | µ |
| -1.61 | -1.61 | -1.6 | -1.49 | ∆ф |
| +2.73 | +2.62 | +2.32 | +2.44 | ∆N |
| +9.77 | +5.53 | +4.32 | +4.45 | ω |
| +4.42 | +4.22 | +3.72 | +3.64 | X |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| MODEL II- β | MODEL II-α | MODEL  C-c-β | MODEL  C-c-α | MODEL  C-b-β | MODEL C-b-α | MODEL  C-a-β | MODEL  C-a-α | property |
| -5.50 | -5.67 | -5.62 | -5.73 | -5.01 | -5.15 | -4.98 | -5.10 | EHOMO(ev) |
| -4.42 | -2.92 | -4.34 | -2.77 | -3.64 | -2.22 | -3.81 | -2.32 | ELUMO(ev) |
| +1.08 | +2.75 | +1.28 | +2.96 | +1.36 | +2.93 | +1.16 | +2.78 | E gap |
| -4.96 | -4.29 | -4.98 | -4.25 | -4.32 | -3.68 | -3.94 | -3.71 | E Fermi |
| +4.42 | +2.92 | +4.34 | +2.77 | +3.64 | +2.22 | +3.81 | +2.32 | A |
| +5.50 | +5.67 | +5.62 | +5.73 | +5.01 | +5.15 | +4.98 | +5.10 | I |
| +0.54 | +1.37 | +0.64 | +1.48 | +0.68 | +1.46 | +0.58 | +1.39 | η |
| +0.92 | +0.72 | +0.77 | +0.33 | +0.73 | +0.34 | +0.85 | +0.35 | S |
| \_4.96 | -4.29 | -4.98 | -4.25 | -4.32 | -3.68 | -4.39 | -3.71 | µ |
| -0.54 | -1.37 | -0.64 | -1.48 | -0.68 | -1.46 | -0.58 | \_1.39 | ∆ф |
| +9.18 | +3.13 | +7.77 | +2.87 | +6.34 | +2.51 | +7.54 | +2.67 | ∆N |
| +22.77 | +13.43 | +19.36 | +6.10 | +13.73 | +4.63 | +16.59 | +2.97 | ω |
| +4.29 | +4.29 | +4.98 | +4.25 | +4.32 | +3.68 | +4.39 | +3.71 | X |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| MODEL IV- β | MODEL IV-α | MODEL  D-c-β | MODEL  D-c-α | MODEL  D-b-β | MODEL  D-b-α | MODEL  D-a-β | MODEL  D-a-α | property |
| -5/82 | -4/79 | -6.13 | -5.16 | -5.70 | -4.93 | -4.97 | -4.66 | E HOMO(ev) |
| -3/28 | -3/07 | -3.61 | -3.37 | -3.25 | -2.99 | -2.70 | -2.58 | E LUMO(ev) |
| +2/53 | +1/71 | +2.51 | +1.79 | +2.45 | +1.93 | +2.27 | +2.08 | E gap |
| -4/55 | -3/93 | -4.87 | -4.27 | -4.48 | -3.96 | +4.97 | -2.62 | E Fermi |
| +3/28 | +3/07 | +3.61 | +3.37 | +3.25 | +2.99 | +2.70 | +2.58 | A |
| +5/82 | +4/79 | +6.13 | +5.16 | +5.70 | +4.93 | +4.97 | +4.66 | I |
| +1/26 | +0/85 | +1.25 | +0.89 | +1.22 | +0.96 | +1.13 | +1.04 | η |
| +0/39 | +0/58 | +0.39 | +0.55 | +0.48 | +0.51 | +0.44 | +0.48 | S |
| -4/55 | -3/93 | -4.87 | -4.27 | -4.48 | -3.96 | -3.83 | -2.62 | µ |
| \_1/26 | +0/85 | -1.25 | -0.89 | -1.22 | -0.96 | -1.13 | -1.04 | ∆ф |
| +3/59 | +4/57 | +3.87 | +4.75 | +3.65 | +4.08 | +3.38 | +2.51 | ∆N |
| +8/19 | +9/00 | +9.45 | +10.16 | +8.19 | +5.10 | +6.47 | +5.44 | ω |
| +4/55 | +3/93 | +4.87 | +4.27 | +4.48 | +3.96 | -3.83 | +2.26 | X |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| MODEL I-β | MODEL I-α | MODEL  E-c-β | MODEL  E-c-α | MODEL  E-b-β | MODEL  E-b-α | MODEL  E-a-β | MODEL  E-a-α | property |
| -5.82 | -5.75 | -6.04 | -6.07 | -5.05 | -4.28 | -4.92 | -4.09 | EHOMO(ev) |
| -3.93 | -2.82 | -4.29 | -3.07 | -2.65 | -2.35 | -2.48 | -2.32 | E LUMO(ev |
| 1.88 | 2.93 | +1.75 | +2.99 | +2.39 | +1.92 | +2.44 | +1.77 | E gap |
| -4.87 | -4.28 | -5.17 | -4.57 | -3.85 | -3.31 | -3.70 | -3.21 | E Fermi |
| 3.93 | 2.82 | +4.29 | +3.07 | +2.65 | +2.35 | +2.48 | +2.32 | A |
| 5.82 | 5.75 | +6.04 | +6.07 | +5.05 | +4.28 | +4.92 | +4.09 | I |
| 0.94 | 1.46 | +0.87 | +1.50 | 1.19 | +0.96 | +1.22 | +0.88 | η |
| 0.52 | 0.34 | +0.57 | +0.33 | 0.41 | +0.51 | +0.40 | +0.56 | S |
| -4.87 | -4.28 | -5.17 | -4.57 | -3.85 | -3.31 | -3.70 | -3.21 | µ |
| -0.94 | -1.46 | -0.87 | -1.50 | -1.19 | -0.96 | -1.22 | -0.88 | ∆ф |
| 5.16 | 2.92 | +5.90 | +3.04 | +3.21 | +3.45 | +3.03 | +3.62 | ∆N |
| 12.61 | 6.26 | +15.26 | +6.97 | +6.18 | +5.70 | +5.62 | +5.81 | ω |
| 4.87 | 4.28 | +5.17 | +4.57 | +3.85 | +3.31 | +3.70 | +3.21 | X |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| MODEL III-β | MODEL III-α | MODEL  F-c-β | MODEL  F-c-α | MODEL  F-b-β | MODEL  F-b-α | MODEL  F-a-β | MODEL  F-a-α | property |
| -5.82 | -5.42 | -6 | -5.62 | -5.21 | -4.80 | -4.93 | -4.02 | **E HOMO(e** |
| -3.15 | -2.86 | -3.32 | -3.04 | -2.53 | -2.13 | -2.45 | -2.45 | **E LUMO(ev** |
| 2.67 | 2.55 | +2.67 | +2.57 | +2.68 | +2.67 | +2.48 | +1.57 | **E gap** |
| -4.48 | -4.14 | -4.66 | -4.33 | -3.87 | -3.46 | -3.69 | -3.23 | **E Fermi** |
| 3.15 | 2.86 | +3.32 | +3.04 | +2.53 | +2.13 | +2.45 | +0.63 | **A** |
| 5.82 | 5.42 | +6 | +5.62 | +5.21 | +4.80 | +4.93 | +4.02 | **I** |
| 1.33 | 1.27 | +1.33 | +1.28 | +1.33 | +1.33 | +1.24 | +2.45 | **η** |
| 0.37 | 0.39 | +0.37 | +0.38 | +0.37 | +0.37 | +0.40 | +0.63 | **S** |
| -4.48 | -4.14 | -4.66 | -4.33 | -3.87 | -3.46 | -3.69 | -3.23 | **µ** |
| -1.33 | -1.27 | -1.33 | -1.28 | -1.33 | -1.33 | -1.24 | -0.78 | **∆ф** |
| 3.35 | 3.24 | +3.49 | +3.36 | +2.89 | +2.59 | +2.97 | +4.14 | **∆N** |
| 7.53 | 6.72 | +8.14 | +7.29 | +5.61 | +4.50 | +5.49 | +6.66 | **ω** |
| 4.48 | 4.14 | +4.66 | +4.43 | +3.87 | +3.46 | +3.69 | +3.23 | **X** |

**Table S3** Comparison of energy of donor-acceptor orbital for A-a to F-c models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | | | E2(Kcal/mol) | | Acceptor(j) | Donor(i) | | Structure | |
| 0.078 | | 0.76 | 9.98 | | σ\*Si1 - C13 | | | Si5 - C16 | | Model A-a |
| 0.057 | | 0.72 | 5.63 | | σ\*Si3 – C14 | | | σSi5 - C16 | |
| 0.025 | | 0.72 | 1.05 | | σ\*Si5 -C16 | | | σSi5 - C16 | |
| 0.077 | | 0.76 | 9.77 | | σ\*Si1- C13 | | | σSi5 - C18 | |
| 0.016 | | 0.53 | 0.53 | | π\*Si9 - C18 | | | σSi5 - C18 | |
| 0.055 | | 0.79 | 5.18 | | σ\*Si9 - C20 | | | σSi5 - C18 | |
| 0.018 | | 0.80 | 0.52 | | σ\*Si1- C13 | | | σSi5 - C24 | |
| 0.045 | | 0.77 | 3.34 | | σ\*Si5 - C16 | | | σSi5 - C24 | |
| 0.039 | | 0.73 | 2.39 | | σ\*Si5-C18 | | | σSi5 - C24 | |
| 0.079 | | 0.75 | 10.40 | | σ\*Si1-C13 | | | σSi5 - C16 | | Model A-b |
| 0.023 | | 0.72 | 5.22 | | σ\*Si3 - C14 | | | σSi5 - C16 | |
| 0.023 | | 0.72 | 0.91 | | σ\*Si5 - C16 | | | σSi5 - C16 | |
| 0.079 | | 0.76 | 10.42 | | σ\*Si1 - C13 | | | σSi5 - C18 | |
| 0.020 | | 0.77 | 0.87 | | σ\*Si5 - C18 | | | σSi5 - C18 | |
| 0.016 | | 0.52 | 0.58 | | π\*Si9 - C18 | | | σSi5 - C18 | |
| 0.018 | | 0.80 | 0.51 | | σ\*Si1- C13 | | | σSi5 - C24 | |
| 0.045 | | 0.77 | 3.22 | | σ\*Si5- C16 | | | σSi5 - C24 | |
| 0.055 | | 0.73 | 0.62 | | σ\*Si8 - C23 | | | σSi5 - C24 | |
| 0.079 | | 0.76 | 10.25 | | σ\*Si1 - C13 | | | σSi5 - C16 | | Model A-c |
| 0.057 | | 0.76 | 5.35 | | σ\*Si3 - C16 | | | σSi5 - C16 | |
| 0.016 | | 0.53 | 0.54 | | π\*Si3 - C16 | | | σSi5 - C16 | |
| 0.079 | | 0.76 | 10.23 | | σ\*Si1- C13 | | | σSi5 - C18 | |
| 0.024 | | 0.73 | 0.99 | | σ\*Si5 - C18 | | | σSi5 - C18 | |
| 0.016 | | 0.53 | 0.57 | | π\*Si9 - C18 | | | σSi5 - C18 | |
| 0.018 | | 0.81 | 0.51 | | σ\*Si1 - C13 | | | σSi5 - C24 | |
| 0.019 | | 0.78 | 3.02 | | σ\*Si6 - C24 | | | σSi5 - C24 | |
| 0.043 | | 0.78 | 0.59 | | σ\*Si8 -C23 | | | σSi5 - C24 | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | E2(Kcal/mol) | | | Acceptor(j) | Donor(i) | Structure |
| 0.042 | 0.79 | 2.74 | | σ\*Si1-C16 | | σSi1-C13 | Model B-a |
| 0.045 | 0.78 | 3.28 | | σ\*Si2-C13 | | σSi1-C13 |
| 0.022 | 0.81 | 0.75 | | σ\*Si2-C14 | | σSi1-C13 |
| 0.021 | 0.73 | 0.78 | | σ\*Si1– C16 | | σSi1-C16 |
| 0.055 | 0.72 | 5.29 | | σ\*Si3-C15 | | σSi1-C16 |
| 0.077 | 0.76 | 9.95 | | σ\*Si5-C24 | | σSi1-C16 |
| 0.020 | 0.75 | 0.87 | | n\*Si1 | | σSi1-C18 |
| 0.078 | 0.72 | 1.00 | | σ\*Si1-C18 | | σSi1-C18 |
| 0.024 | 0.50 | 10.11 | | σ\*Si5-C24 | | σSi1-C18 |
| 0.046 | 0.78 | 3.36 | | σ\*Si1-C18 | | σSi1-C13 | Model B-b |
| 0.045 | 0.78 | 0.52 | | σ\*Si2-C19 | | σSi1-C13 |
| 0.018 | 0.79 | 3.24 | | σ\*Si12-C13 | | σSi1-C13 |
| 0.022 | 0.73 | 0.85 | σ\*Si1-C16 | | | σSi1-C16 |
| 0.055 | 0.72 | 5.45 | σ\*Si3-C15 | | | σSi1-C16 |
| 0.078 | 0.76 | 9.94 | σ\*Si5-C24 | | | σSi1-C16 |
| 0.023 | 0.72 | 0.88 | σ\*Si1-C18 | | | σSi1-C18 |
| 0.077 | 0.72 | 9.87 | σ\*Si5-C24 | | | σSi1-C18 |
| 0.056 | 0.76 | 5.15 | σ\*Si9-C21 | | | σSi1-C18 |
| 0.053 | 0.76 | 4.65 | σ\*Si1-C18 | | | σSi1-C13 | Model B-c |
| 0.016 | 0.50 | 0.54 | π\*Si11-C19 | | | πSi1-C13 |
| 0.087 | 0.28 | 33.64 | π\*Si12-C20 | | | πSi1-C13 |
| 0.017 | 0.71 | 0.51 | σ\*Si1-C16 | | | σSi1-C16 |
| 0.048 | 0.74 | 3.88 | σ\*Si3–C16 | | | σSi1-C16 |
| 0.064 | 0.74 | 6.87 | σ\*Si5-C24 | | | σSi1-C16 |
| 0.018 | 0.71 | 3.41 | σ\*Si1-C16 | | | σSi1-C18 |
| 0.061 | 0.74 | 0.55 | σ\*Si1-C18 | | | σSi1-C18 |
| 0.044 | 0.70 | 6.26 | σ\*Si5-C24 | | | σSi1-C18 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | | E2(Kcal/mol) | | | Acceptor(j) | Donor(i) | | Structure |
| 0.059 | | 0.77 | | 2.89 | σ\*Si1–C12 | | | σC17–B34 | Model C-a |
| 0.049 | | 0.74 | | 2.02 | σ\*Si3–C15 | | | σC17–B34 |
| 0.025 | | 1.00 | | 0.37 | σ\*C24–C25 | | | σC17–B34 |
| 0.041 | | 0.83 | | 1.07 | σ\*C24–C25 | | | σC25–B34 |
| 0.018 | | 0.45 | | 0.39 | σ\*C25– B34 | | | σC25–B34 |
| 0.062 | | 0.53 | | 3.40 | n\*B34 | | | σSi5–C23 |
| 0.035 | | 1.07 | | 0.55 | n\*B34 | | | σC24–O26 |
| 0.068 | | 0.77 | | 3.72 | σ\*Si1– C12 | | | σC15–B34 | Model C-b |
| 0.051 | | 0.55 | | 2.75 | π\*Si1–C12 | | | σC15–B34 |
| 0.027 | | 0.73 | | 0.63 | σ\*Si1–C17 | | | σC15–B34 |
| 0.058 | | 0.51 | | 3.29 | n\*B34 | | | σC17–B34 |
| 0.067 | | 0.77 | | 3.67 | σ\*Si1–C12 | | | σC17–B34 |
| 0.025 | | 0.93 | | 0.42 | σ\*C23–B34 | | | σC17–B34 |
| 0.020 | | 0.82 | | 0.29 | σ\*Si1–C12 | | | σC23–B34 |
| 0.055 | | 0.64 | | 2.62 | π\*Si5–C14 | | | σC23–B34 |
| 0.045 | | 0.59 | | 1.97 | π\*Si7–C20 | | | σC23–B34 |
| 0.027 | | 0.72 | | 0.60 | σ\*Si1–C17 | | | σC15–B34 | Model C-c |
| 0.044 | | 0.72 | | 1.64 | σ\*Si3–C13 | | | σC15–B34 |
| 0.049 | | 0.75 | | 2.05 | σ\*Si3–C15 | | | σC15–B34 |
| 0.017 | | 0.57 | | 0.26 | n\*B34 | | | σC17–B34 |
| 0.020 | | 0.86 | | 3.15 | σ\*Si1–C12 | | | σC17– B34 |
| 0.021 | | 0.88 | | 0.30 | σ\*C23–B34 | | | σC17– B34 |
| 0.025 | | 0.74 | | 0.52 | σ\*Si1–C15 | | | σC23–B34 |
| 0.038 | | 0.76 | | 1.17 | σ\*Si5–C23 | | | σC23–B34 |
| 0.062 | | 0.76 | | 0.30 | σ\*C17–B34 | | | σC23–B34 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | | E2(Kcal/mol) | | | Acceptor(j) | Donor(i) | Structure |
| 0.066 | | 0.38 | | 6.55 | π\*Si3-C13 | | πC15-N34 | Model D-a |
| 0.060 | | 0.25 | | 6.00 | π\*C15-N 34 | | πC15-N34 |
| 0.018 | | 0.68 | | 0.29 | σ\*C17-N 34 | | πC15-N34 |
| 0.056 | | 1.01 | | 1.87 | σ\*Si3-C15 | | σC17-N34 |
| 0.029 | | 1.01 | | 0.51 | σ\*Si8-C17 | | σC17-N34 |
| 0.052 | | 1.17 | | 1.43 | σ\*C23-N34 | | σC17-N34 |
| 0.022 | | 1.08 | | 0.26 | σ\*Si3- C15 | | σC23-N34 |
| 0.044 | | 1.19 | | 1.28 | σ\*C15-N 34 | | σC23-N34 |
| 0.049 | | 1.17 | | 1.03 | σ\*C17- N 34 | | σC23-N34 |
| 0.020 | | 0.93 | | 0.26 | σ\* Si3- C13 | | σC23-N34 | Model D-b |
| 0.049 | | 0.89 | | 1.65 | σ\* Si7- C23 | | σC15 - N34 |
| 0.054 | | 1.07 | | 1.89 | σ\* Si8- C17 | | σC15-N34 |
| 0.047 | | 0.94 | | 1.43 | σ\*Si1- C12 | | σC17- N34 |
| 0.021 | | 0.93 | | 0.29 | σ\*Si1- C17 | | σC17-N34 |
| 0.047 | | 0.91 | | 1.52 | σ\*Si5- C 23 | | σC17-N34 |
| 0.025 | | 0.99 | | 0.37 | σ\*Si1- C15 | | σC23-N34 |
| 0.023 | | 1.03 | | 0.51 | σ\*Si1- C17 | | σC23-N34 |
| 0.029 | | 0.93 | | 0.31 | σ\*Si5- C14 | | σC23-N34 |
| 0.020 | | 0.94 | | 0.50 | σ\*Si3- C15 | | σC15-N34 | Model D-c |
| 0.028 | | 0.94 | | 1.80 | σ\*Si8- C17 | | σC15-N34 |
| 0.053 | | 1.01 | | 0.28 | σ\*C17- N 34 | | σC15-N34 |
| 0.021 | | 0.96 | | 1.71 | σ\*Si3- C15 | | σC17-N34 |
| 0.052 | | 0.91 | | 1.48 | σ\*Si5- C23 | | σC17-N34 |
| 0.047 | | 1.01 | | 0.26 | σ\*C15- N 34 | | σC23-N34 |
| 0.020 | | 1.07 | | 0.25 | σ\*Si5 - C14 | | σC23-N34 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | E2(Kcal/mol) | | Acceptor(j) | Donor(i) | Structure |
| 0.065 | 0.65 | 3.97 | σ\*Si1-C13 | | σSi5-B34 | Model E-a |
| 0.051 | 0.66 | 2.42 | σ\*Si5-C23 | | σSi5-B34 |
| 0.016 | 0.62 | 0.25 | σ\*Si6- C22 | | σSi5-B34 |
| 0.038 | 0.38 | 2.15 | n\*B34 | | σSi3-B34 |
| 0.046 | 0.39 | 3.24 | σ\*Si1-C13 | | σSi3-B34 |
| 0.016 | 0.58 | 0.27 | σ\*Si5– C17 | | σSi3-B34 |
| 0.063 | 0.61 | 0.58 | σ\*Si3-C15 | | σSi1-B34 |
| 0.022 | 0.66 | 3.73 | σ\*Si5-C23 | | σSi1-B34 |
| 0.025 | 0.64 | 0.47 | σ\*Si5-B34 | | σSi1-B34 |
| 0.026 | 0.64 | 2.56 | σ\*Si3-C15 | | σSi1-B34 | Model E-b |
| 0.030 | 0.44 | 0.59 | σ\*Si5-C17 | | σSi1-B34 |
| 0.063 | 0.66 | 4.34 | σ\*Si5-C23 | | σSi1-B34 |
| 0.042 | 0.38 | 3.14 | n\*B34 | | σSi3-B34 |
| 0.051 | 0.41 | 2.88 | π\*Si1-C13 | | σSi3-B34 |
| 0.018 | 0.67 | 0.25 | σ\*Si4-C16 | | σSi3-B34 |
| 0.064 | 0.66 | 4.53 | σ\*Si1-C13 | | σSi5-B34 |
| 0.019 | 0.66 | 0.29 | σ\*Si1-B34 | | σSi5-B34 |
| 0.048 | 0.61 | 1.47 | σ\*Si5-C23 | | σSi5-B34 |
| 0.051 | 0.62 | 2.56 | σ\*Si3-C15 | | σSi1-B34 | Model E-c |
| 0.025 | 0.63 | 0.59 | σ\*Si3-B34 | | σSi1-B34 |
| 0.067 | 0.65 | 4.34 | σ\*Si5-C23 | | σSi1-B34 |
| 0.058 | 0.68 | 3.14 | σ\*Si3 - C14 | | σSi3- B34 |
| 0.055 | 0.65 | 2.88 | σ\*Si3 - C15 | | σSi3- B34 |
| 0.017 | 0.71 | 0.25 | σ\*Si4 -C16 | | σSi3- B34 |
| 0.039 | 0.65 | 4.53 | σ\*Si1- C13 | | σSi5 - B34 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| F(i,j) | E(j)-E(i) | | E2(Kcal/mol) | | Acceptor(j) | Donor(i) | Structure |
| 0.188 | 0.86 | 3.28 | | n\*Si1 | | σSi8-N34 | Model F-a |
| 0.023 | 1.03 | 0.33 | | σ\*Si8-N34 | | σSi8-N34 |
| 0.081 | 0.40 | 9.90 | | π\*Si1-C12 | | nN34 |
| 0.038 | 0.42 | 1.99 | | π\*Si1-C12 | | nN34 |
| 0.048 | 0.60 | 2.11 | | σ\*Si1-C32 | | nN34 |
| 0.063 | 0.35 | 2.82 | | π\*Si8-C17 | | nN34 |
| 0.057 | 0.53 | 3.39 | | σ\*Si8-C17 | | nN34 |
| 0.015 | 0.39 | 0.35 | | π\*Si8– C17 | | nN34 |
| 0.204 | 0.87 | 27.69 | | n\*Si3 | | σSi1-N34 | Model F-b |
| 0.022 | 1.01 | 0.29 | | σ\*Si3- C14 | | σSi1-N34 |
| 0.071 | 0.37 | 7.98 | | n\*Si3 | | nN34 |
| 0.069 | 0.43 | 7.55 | | n\*Si3 | | nN34 |
| 0.018 | 0.61 | 0.30 | | n\*Si1-C13 | | nN34 |
| 0.058 | 0.33 | 6.32 | | n\*Si1-C13 | | nN34 |
| 0.019 | 0.39 | 0.56 | | n\*Si1-C13 | | nN34 |
| 0.027 | 0.88 | 52.96 | | n\*Si5 | | σSi1N34 | Model F-c |
| 0.067 | 0.85 | 3.18 | | π\*Si5-C17 | | σSi1N34 |
| 0.282 | 1.06 | 0.39 | | σ\*Si9-C17 | | σSi1N34 |
| 0.024 | 0.35 | 0.96 | | n\*Si3 | | nN34 |
| 0.059 | 0.29 | 7.63 | | n\*Si3 | | nN34 |
| 0.190 | 0.44 | 51.53 | | n\*Si3 | | nN34 |
| 0.055 | 0.56 | 2.94 | | σ\*Si5-C17 | | nN34 |
| 0.018 | 0.51 | 0.32 | | σ\*Si5-C17 | | nN34 |
| 0.016 | 0.33 | 0.47 | | σ\*Si5-C17 | | nN34 |

**Table S4**The NBO and Milliken charge around Glycine for A-a to F-c models

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ∆P NBO | ∆P Muliken | Model | ∆P NBO | ∆P Muliken | Model |
| +0.216 | +0.320 | **D-a** | +0.213 | +0.319 | **A-a** |
| -0.503 | -0.181 | **D-b** | +0.185 | +0.269 | **A-b** |
| -0.005 | -0.016 | **D-c** | +0.207 | +0.288 | **A-c** |
| +0.307 | +0.325 | **E-a** | +0.222 | +0.333 | **B-a** |
| +0.306 | +0.334 | **E-b** | +0.184 | +0.363 | **B-b** |
| +0.007 | +0.005 | **E-c** | +0.171 | +0.269 | **B-c** |
| +0.212 | +0.338 | **F-a** | +0.307 | +0.269 | **C-a** |
| +0.193 | +0.289 | **F-b** | +0.215 | +0.327 | **C-b** |
| +0.010 | +0.025 | **F-c** | -0.237 | -0.157 | **C-c** |