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SUPPLEMENTARY INFORMATION

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Calculations predict a stable molecular crystal of N_8

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I. STRUCTURES OF DIFFERENT FORMS OF SOLID NITROGEN

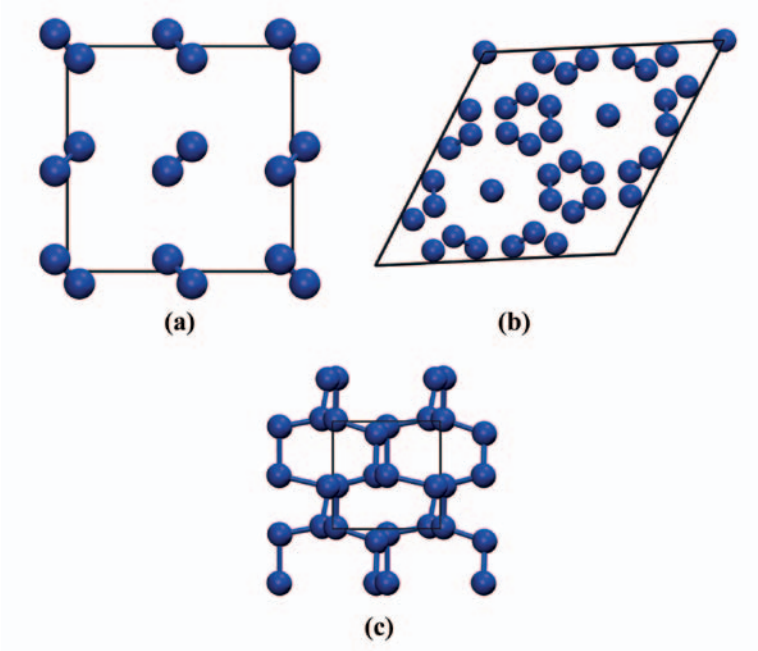

FIG. S1: Structures of different solid forms of nitrogen: α-N_2 (a), ϵ-N_2 (b), and cg-N (c).

II. COMPUTATIONAL DETAILS

For solid calculations, we employed the QuantumEspresso 4.3.1 [1] package. All other calculations were performed using Q-Chem 4.0[2]. Both methods were chosen because of the accurate description of dispersion interactions, which are of crucial importance in molecular crystals. The aug-cc-pVDZ basis set was employed in these calculations[3]. Default criteria for convergence of the SCF procedure and geometry optimizations were used. Natural Bond Orbital (NBO) analysis has been used to analyze bonding[4–6].

All Cartesian geometries and relevant energies are given below.

III. UNIT CELL STRUCTURES AND COHESIVE ENERGIES

Table S1 summarizes the computed structural parameters and cohesive energies computed using different PBC PW-DFT methods. Importantly, all optimization converge to a similar-type structures. The variations in structural parameters are reasonably small, e.g., no more than 10 % in V_0. As expected, energetics is more sensitive to the functional, e.g., BLYP-D predicts twice smaller cohesive energy. Importantly, VDW-DF predict even stronger cohesive energy than PBE-D.

TABLE S1: Unit cell parameters and cohesive energies computed by PBC PW-DFT.

Method	a, Å	b, Å	c, Å	α	β	γ	V_0, Å^3	E_c, kJ/mol
PBE-D	10.72	4.53	6.90	91.5	84.9	45.9	14.89	41.1
BLYP-D	10.59	4.40	6.42	89.2	83.3	44.1	12.86	24.4
VDW-DF	10.83	4.67	7.05	88.4	81.7	47.4	16.17	61.0

IV. GEOMETRY OPTIMIZATION USING DIFFERENT DISTORTED STRUCTURES

To investigate the sensitivity of the computed structures to the starting geometries, we performed series of calculations in which unit cell structures were reoptimized starting from various distorted geometries as described below. These calculations were performed using PBC PW PBE-D. All these calculations, the optimizations converged to the same unit cell structure as in the original calculation (initiated from four N_4). The following displacement have been tested (see Fig. S2 for the respective structures):

- Elongation of the N2-N3 bond in the E monomer by 0.5 Å;
- Elongation of the N2-N3 bond in the Z monomer by 0.5 Å;
- Rotation of the dihedral N1-N2-N3-N4 angle by -40° in the E monomer;
- Rotation of the dihedral N1-N2-N3-N4 angle by -40° in the E monomer.

V. MOLECULAR STRUCTURES AND ENERGETICS

Optimized structures of the N_8 monomers and relevant total energies are given below. Fig. S3a shows relevant structural parameters at the PBE and ωB97X-D levels of theory. We observe that the maximum variation in bond length is 0.1 Å for the N_2-N_3 bond for the EZE isomer. However, most bond lengths are very similar (less than 0.05 Å difference) using both methods. The NBO analysis yields very similar results to those reported in Ref. [7]. Fig. S3b compares NBO charges computed by PBE and ωB97X-D. We observe that both functionals produce very similar charge distributions. Thus, in this case, the effect of self-interaction error (which may affect quality of the PBE results) is not substantial.

In addition, we computed NBO charges for the Z monomer at minimum geometry from PBE-D calculations using the CCSD level of theory. Table S2 below summarizes the results

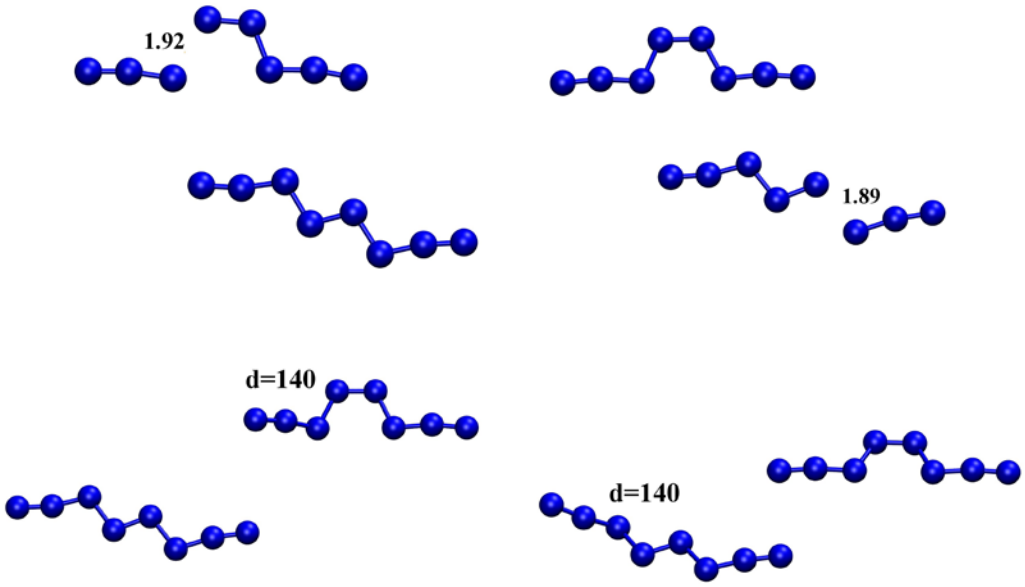

FIG. S2: Different distorted unit cell structures used as starting points in geometry optimizations.

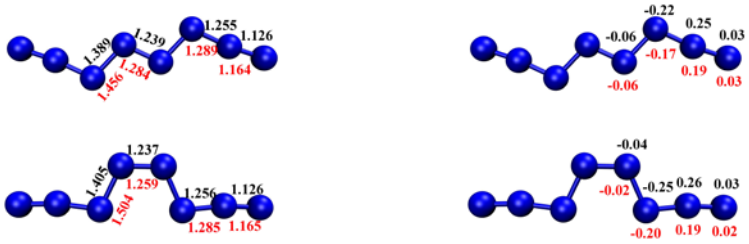

FIG. S3: Optimized structures of N_8 monomers and comparison of bond lengths and NBO partial charges computed using ωB97X-D (top, black) and PBE-D (bottom, red).

of NBO analysis of the CCSD and PBE-D densities computed with the cc-pVDZ basis set. The raw outputs are given in Section X. As one can see, the bond orders (BO, computed as 1/2 of the NBO populations assigned to the particular bond) and partial charges are in excellent agreement suggesting that PBE-D captures important details of the electronic structure of N_8. The bonding picture given by NBO can be best described by the Lewis structure shown in Fig. 1 of the main paper.

VI. CLUSTER CALCULATIONS

Fig. S4 shows optimized structures and binding energies for several dimers of N_8. Structures and basis-set superposition error (BSSE) corrected binding energies are computed using ωB97X-D/aug-cc-pVDZ. Zero-point energy (ZPE) correction for the binding energies

TABLE S2: Natural atomic charges and bond orders (BO) from the NBO analysis of the PBE-D and CCSD densities. Atom numbering is the same as in Fig. 1 of the main paper.

Method	N3 charge	N4 charge	N1N2 BO	N2N3 BO	N3N4 BO	N4N5 BO
PBE-D	-0.20	+0.20	1.98	0.96	1.00	2.99
CCSD	-0.27	+0.24	1.93	0.95	0.98	2.90

TABLE S3: BSSE corrected binding energies (kcal/mol) of N_4 clusters. ZPE correction is not included.

Parallel Dimer	Tilted Dimer	Tetramer	Method
-1.004	-1.705	-8.838	RI-MOS-MP2/aug-cc-pVDZ
-0.753	-1.610	-7.316	ωB97X-D/aug-cc-pVDZ

are not included. We could not locate a true minimum on the PES for a dimer of the EZE isomer.

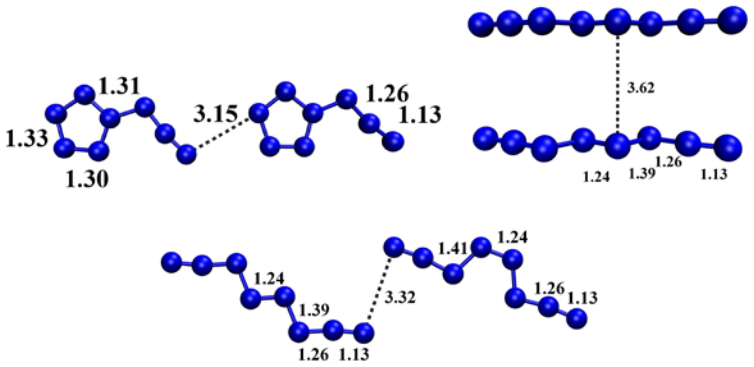

FIG. S4: Optimized structures of several N_8 dimers. The respective binding energies are 1.73 kcal/mol, 0.97 kcal/mol, and 0.36 kcal/mol.

A. Calculations of N_4 clusters

Our initial plan was to investigate whether N_4 can form a stable solid. Thus, we analyzed interactions in N_4 dimers and a tetramer. Fig. S5 shows optimized structures of two N_4 dimers (parallel and tilted configurations) and a tetramer. The geometries computed with ωB97X-D/aug-cc-pVDZ and RI-MOS-MP2/aug-cc-VDZ are very similar. The binding energies for the structures are summarized in Table S3. We note that the binding energies are reasonably large (even larger than in the N_8 dimers), and that there is a non-additive effect in the tetramer, which suggests the existence of a stable solid structure. Yet, when we attempted to optimize a unit cell composed of four N_4 units, the structure converged to the unit cell with two N_8 molecules.

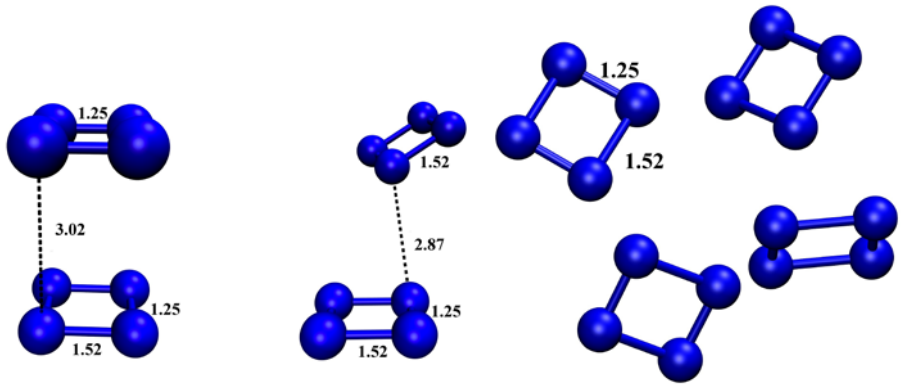

FIG. S5: Structures of D_{2h} N_4 dimers at a tetramer computed by ωB97X-D/aug-cc-pVDZ.

VII. COHESIVE ENERGIES

TABLE S4: Lattice constants and cohesive energies for α-N_2, α-CO_2, and β-acetonitrile (ACN). All calculated values are not zero point energy (ZPE) corrected.

Species	Lattice Constants, Å	Volume, Å^3	Lattice Energy, kJ/mol
N_2 exp.	5.644	179.788	8.30[a] (6.92[b])
N_2 calc.	5.486 (-2.88%)	165.14179 (-8.15%)	8.30
CO_2 exp.	5.554	171.324	26.255[c]
CO_2 calc.	5.638 (1.51%)	179.215 (4.61%)	24.645
ACN exp.	6.0717, 5.2319, 7.7779	247.08[d]	
ACN calc.	5.763 (-5.08%), 5.100 (-2.52%), 7.553 (-2.89%)	221.996 (-10.15%)	53.013

[a] Ref. [8]
[b] Ref. [9]
[c] Ref. [10]
[d] Ref. [11]

The lattice parameters and lattice energy obtained in this study for the α-N_2, α-CO_2, and β-ACN are shown in Table VII and are compared to the experimental values [8–11]. Since α N_2 and CO_2 have an FCC structure, only the volume and lattice vector a are shown. For acetonitrile, all three lattice parameters are given. Table VII shows that the lattice constant obtained for N_2 is in very good agreement with the experiment. In the lattice energy column for N_2, the value shown in parentheses is the experimental value for the sublimation enthalpy. In order to compare this value to the cohesive energy the ZPE must be taken into account. Using high level methods [8] Erba *et. al* calculated the ZPE correction to be 1.4 kJ/mol. Thus, the cohesive energy of solid N_2 calculated in this study (8.3 kJ/mol) is in excellent agreement with the ZPE-corrected experimental value. For CO_2, we obtain a lattice energy of 24.645 kJ/mol, which is also in very good agreement with the experimental value[10]. For acetonitrile, good agreement with experiment is also seen for lattice parameters [11]. However, to the best of our knowledge, cohesive energy data for β-ACN is not available and only calculated value is presented.

VIII. PRESSURE DEPENDENCE AND THERMODYNAMIC STABILITY

TABLE S5: Total electronic enthalpies (eV/atom) and volume per atom (Å^3) of N_8 and cg-N solids at different pressures computed with PBE-D.

P, GPa	H(N_8)	H(cg-N)	ΔH/atom, eV	V_0 (N_8)	V_0 (cg-N)
ambient	-383.138 304	-382.611 042	-0.5274	14.8919	6.7670
5	-382.750 500	-382.408 291	-0.3422	11.2648	6.6525
20	-381.829 049	-381.800 362	-0.0287	8.8970	6.3476
40	-380.806 789	-381.028 772	0.2220	7.6300	6.0264
50	-380.343 865	-380.656 870	0.3130	7.2217	5.8923

Table S5 presents enthalpies of N_8 solid and cg-N form computed by PW-DFT/PBE-D. These results are shown in Fig. 3 of the main manuscript. The results for other forms of nitrogen are taken from Ref. [12]. These enthalpies do not include ZPE correction. To estimates the magnitude of ZPE contribution, we computed ZPE correction at 4 different pressures (5, 20, 40, and 50 GPa) and found that including ZPE leads to slight additional stabilization of N_8 versus cg-N; however, the magnitude of the effect is small, as illustrated in Fig. S6a. Finally, to estimate entropic contributions, we estimated entropy for both solids using the Debye solid model. We found that the contribution of TΔS term is much smaller (about 1% or less) than their enthalpy differences.

To estimate how sensitive the results are to the level of theory, we computed the enthalpies using two alternative functionals (BLYP-D and vdw-DFT). Whereas the pressure for phase transition depends on the method, the overall trend is robust, as illustrated in Fig. S6b which shows pressure dependence of the enthalpy difference relative to cg-N calculated at three different levels of theory.

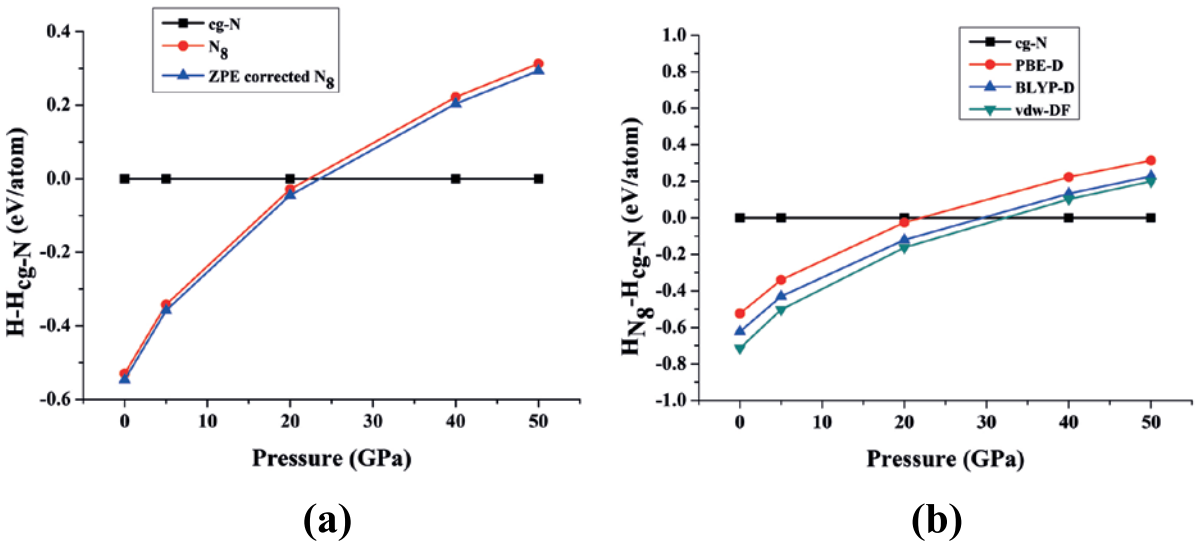

FIG. S6: Pressure dependence of the enthalpy per nitrogen atom relative to the cg-N form computed using different PBC PW-DFT methods.

Finally, Fig. S7 shows enthalpy versus volume dependence of the two forms.

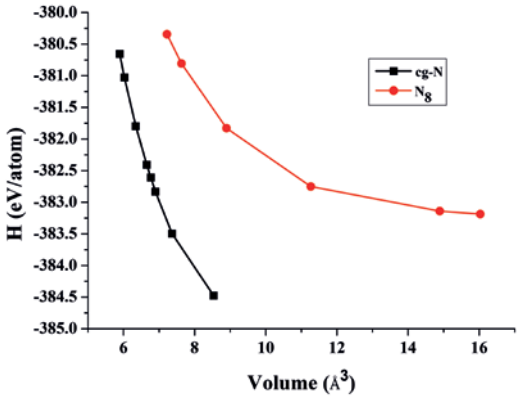

FIG. S7: Volume dependence of the enthalpy per nitrogen atom of solid N_8 and the cg-N form computed using PW-PBE-D.

IX. VIBRATIONAL ANALYSIS

Below are give the vibrational frequencies and IR intensities of the monomers and solid using all different methods. We note that the agreement between different methods is reasonable. This supports the validity of the PW-PBE-D method for solid calculations. The PW-PBE-D results for the solid are very similar to the spectrum computed for the isolated monomers.

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X. NBO ANALYSIS

Below we report the results of the NBO analysis for N_8 (structure optimized at the PBE-D/aug-cc-pVDZ level) using PBE-D and CCSD densities computed with the cc-pVDZ basis.

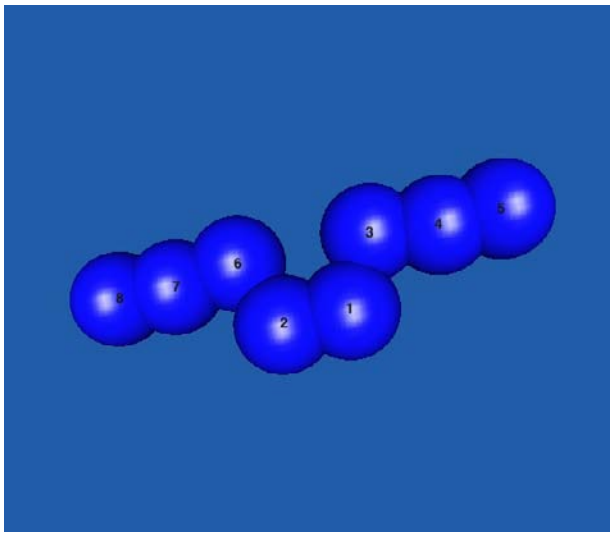

FIG. S8: Atom indexing in the NBO output

PBE-D/cc-pVDZ

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
N 1	-0.01396	1.99956	4.98540	0.02900	7.01396
N 2	-0.01397	1.99956	4.98541	0.02900	7.01397
N 3	-0.20024	1.99945	5.17776	0.02303	7.20024
N 4	0.19823	1.99944	4.77495	0.02738	6.80177
N 5	0.01597	1.99966	4.95993	0.02443	6.98403
N 6	-0.20022	1.99945	5.17774	0.02303	7.20022
N 7	0.19825	1.99944	4.77493	0.02738	6.80175
N 8	0.01593	1.99966	4.95998	0.02443	6.98407
* Total *	0.00000	15.99622	39.79609	0.20769	56.00000

```
.....................................................................
    (Occupancy)   Bond orbital/ Coefficients/ Hybrids
---------------------------------------------------------------------------
  1. (1.98677) BD ( 1) N  1- N  2
             ( 50.00%)   0.7071* N  1 s( 31.57%)p 2.16( 68.21%)d 0.01(  0.23%)
```

```
                                          0.0000 -0.5590 -0.0564 -0.0003  0.0000
                                         -0.0877  0.0271  0.8198  0.0401  0.0000
                                          0.0000  0.0170  0.0075 -0.0442
              ( 50.00%)   0.7071* N  2 s( 31.57%)p 2.16( 68.20%)d 0.01(  0.23%)
                                          0.0000 -0.5590 -0.0564 -0.0003  0.0000
                                         -0.0877  0.0271 -0.8198 -0.0401  0.0000
                                          0.0000 -0.0170  0.0075 -0.0442
 2. (1.97091) BD ( 2) N  1- N  2
              ( 50.00%)   0.7071* N  1 s(  0.00%)p 1.00( 99.71%)d 0.00(  0.29%)
                                          0.0000 -0.0001  0.0000  0.9985  0.0067
                                         -0.0011  0.0000  0.0002  0.0000  0.0224
                                         -0.0486  0.0001  0.0000  0.0000
              ( 50.00%)   0.7071* N  2 s(  0.00%)p 1.00( 99.71%)d 0.00(  0.29%)
                                          0.0000 -0.0001  0.0000  0.9985  0.0067
                                         -0.0011  0.0000 -0.0002  0.0000  0.0224
                                          0.0486 -0.0001  0.0000  0.0000
 3. (1.90627) BD ( 1) N  1- N  3
              ( 48.41%)   0.6958* N  1 s( 14.95%)p 5.68( 84.86%)d 0.01(  0.19%)
                                          0.0002  0.3862  0.0191  0.0009  0.0000
                                          0.8502  0.0017  0.3538  0.0238  0.0001
                                          0.0000  0.0120 -0.0392 -0.0144
              ( 51.59%)   0.7183* N  3 s( 15.20%)p 5.57( 84.62%)d 0.01(  0.18%)
                                         -0.0007  0.3894  0.0178 -0.0011  0.0000
                                         -0.8362 -0.0076 -0.3829 -0.0187  0.0001
                                          0.0000  0.0037 -0.0390 -0.0168
 4. (1.90627) BD ( 1) N  2- N  6
              ( 48.41%)   0.6958* N  2 s( 14.95%)p 5.68( 84.86%)d 0.01(  0.19%)
                                          0.0002  0.3862  0.0191  0.0009  0.0000
                                          0.8502  0.0017 -0.3538 -0.0238  0.0001
                                          0.0000 -0.0120 -0.0392 -0.0144
              ( 51.59%)   0.7183* N  6 s( 15.20%)p 5.57( 84.62%)d 0.01(  0.18%)
                                         -0.0007  0.3894  0.0178 -0.0011  0.0000
                                         -0.8362 -0.0076  0.3829  0.0187  0.0001
                                          0.0000 -0.0037 -0.0390 -0.0168
 5. (1.99339) BD ( 1) N  3- N  4
              ( 43.27%)   0.6578* N  3 s( 23.22%)p 3.29( 76.52%)d 0.01(  0.26%)
                                          0.0000  0.4791  0.0521 -0.0010  0.0000
                                         -0.1697  0.0194  0.8574  0.0290  0.0001
                                         -0.0001 -0.0247 -0.0098  0.0433
              ( 56.73%)   0.7532* N  4 s( 49.42%)p 1.02( 50.52%)d 0.00(  0.06%)
                                          0.0000  0.7028 -0.0181  0.0011  0.0000
                                          0.0264  0.0158 -0.7101 -0.0046  0.0000
                                         -0.0001 -0.0028 -0.0021  0.0252
 6. (1.99910) BD ( 1) N  4- N  5
              ( 56.33%)   0.7505* N  4 s( 49.40%)p 1.02( 50.53%)d 0.00(  0.07%)
                                         -0.0001  0.7026  0.0185 -0.0012 -0.0001
                                         -0.1686  0.0025  0.6893  0.0415  0.0000
```

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                                          -0.0001 -0.0037 -0.0002  0.0256
              ( 43.67%)   0.6609* N  5 s( 28.75%)p 2.47( 70.92%)d 0.01(  0.33%)
                                           0.0000  0.5313  0.0723  0.0008  0.0000
                                          -0.2006 -0.0057 -0.8174 -0.0295  0.0000
                                          -0.0001  0.0144 -0.0011  0.0559
 7. (1.99044) BD ( 2) N  4- N  5
              ( 52.89%)   0.7273* N  4 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)
                                           0.0000 -0.0001  0.0000  0.9992 -0.0094
                                          -0.0014  0.0000  0.0014  0.0000  0.0041
                                           0.0384  0.0000  0.0000  0.0001
              ( 47.11%)   0.6863* N  5 s(  0.00%)p 1.00( 99.60%)d 0.00(  0.40%)
                                           0.0000  0.0000  0.0000  0.9979  0.0158
                                          -0.0014  0.0000  0.0013  0.0000 -0.0012
                                          -0.0631  0.0001  0.0001 -0.0001
 8. (1.97819) BD ( 3) N  4- N  5
              ( 58.20%)   0.7629* N  4 s(  1.06%)p93.01( 98.84%)d 0.09(  0.10%)
                                          -0.0002  0.1018  0.0160  0.0012  0.0000
                                           0.9846 -0.0169  0.1366  0.0001  0.0000
                                           0.0000  0.0310 -0.0048  0.0034
              ( 41.80%)   0.6465* N  5 s(  1.14%)p86.57( 98.44%)d 0.38(  0.43%)
                                           0.0000  0.1052  0.0174  0.0016  0.0001
                                           0.9771  0.0266 -0.1699 -0.0099  0.0001
                                          -0.0001 -0.0639  0.0009  0.0132
 9. (1.99339) BD ( 1) N  6- N  7
              ( 43.27%)   0.6578* N  6 s( 23.22%)p 3.29( 76.52%)d 0.01(  0.26%)
                                           0.0000  0.4791  0.0521 -0.0010  0.0000
                                          -0.1697  0.0194 -0.8574 -0.0290  0.0001
                                           0.0001  0.0247 -0.0098  0.0433
              ( 56.73%)   0.7532* N  7 s( 49.42%)p 1.02( 50.52%)d 0.00(  0.06%)
                                           0.0000  0.7028 -0.0181  0.0011  0.0000
                                           0.0264  0.0158  0.7101  0.0046  0.0000
                                           0.0001  0.0028 -0.0021  0.0252
10. (1.99910) BD ( 1) N  7- N  8
              ( 56.33%)   0.7505* N  7 s( 49.40%)p 1.02( 50.53%)d 0.00(  0.07%)
                                          -0.0001  0.7026  0.0185 -0.0012 -0.0001
                                          -0.1686  0.0025 -0.6894 -0.0415  0.0000
                                           0.0001  0.0037 -0.0002  0.0256
              ( 43.67%)   0.6609* N  8 s( 28.75%)p 2.47( 70.92%)d 0.01(  0.33%)
                                           0.0000  0.5313  0.0723  0.0008  0.0000
                                          -0.2006 -0.0057  0.8174  0.0295  0.0000
                                           0.0001 -0.0144 -0.0011  0.0559
11. (1.99044) BD ( 2) N  7- N  8
              ( 52.89%)   0.7273* N  7 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)
                                           0.0000 -0.0001  0.0000  0.9992 -0.0094
                                          -0.0014  0.0000 -0.0014  0.0000  0.0041
                                          -0.0384  0.0000  0.0000  0.0001
              ( 47.11%)   0.6863* N  8 s(  0.00%)p 1.00( 99.60%)d 0.00(  0.40%)
```

```
                                      0.0000  0.0000  0.0000  0.9979  0.0158
                                     -0.0014  0.0000 -0.0013  0.0000 -0.0012
                                      0.0631 -0.0001  0.0001 -0.0001
 12. (1.97819) BD ( 3) N  7- N  8
             ( 58.20%)   0.7629* N  7 s(  1.06%)p93.01( 98.84%)d 0.09(  0.10%)
                                     -0.0002  0.1018  0.0160  0.0012  0.0000
                                      0.9846 -0.0169 -0.1366 -0.0001  0.0000
                                      0.0000 -0.0310 -0.0048  0.0034
             ( 41.80%)   0.6465* N  8 s(  1.14%)p86.57( 98.44%)d 0.38(  0.43%)
                                      0.0000  0.1052  0.0173  0.0016  0.0001
                                      0.9771  0.0266  0.1699  0.0099  0.0001
                                      0.0001  0.0639  0.0009  0.0132
 13. (1.99956) CR ( 1) N  1           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0001  0.0000  0.0000  0.0000
                                     -0.0003  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 14. (1.99956) CR ( 1) N  2           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0001  0.0000  0.0000  0.0000
                                     -0.0003  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 15. (1.99945) CR ( 1) N  3           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0000  0.0000  0.0000  0.0000
                                     -0.0008  0.0000 -0.0002  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 16. (1.99944) CR ( 1) N  4           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0002  0.0000  0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 17. (1.99966) CR ( 1) N  5           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0005  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0003  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 18. (1.99945) CR ( 1) N  6           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0000  0.0000  0.0000  0.0000
                                     -0.0008  0.0000  0.0002  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 19. (1.99944) CR ( 1) N  7           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0002  0.0000 -0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 20. (1.99966) CR ( 1) N  8           s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0005  0.0000  0.0000  0.0000
                                      0.0000  0.0000 -0.0003  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
 21. (1.90228) LP ( 1) N  1           s( 53.72%)p 0.86( 46.20%)d 0.00(  0.08%)
                                     -0.0001  0.7324 -0.0271 -0.0006  0.0000
                                     -0.5153  0.0171  0.4423 -0.0254  0.0000
```

```
                                          0.0000  0.0249  0.0118 -0.0035
 22. (1.90228) LP ( 1) N  2             s( 53.72%)p 0.86( 46.20%)d 0.00(  0.08%)
                                         -0.0001  0.7324 -0.0271 -0.0006  0.0000
                                         -0.5153  0.0171 -0.4423  0.0254  0.0000
                                          0.0000 -0.0249  0.0118 -0.0035
 23. (1.84512) LP ( 1) N  3             s( 61.80%)p 0.62( 38.13%)d 0.00(  0.07%)
                                          0.0004  0.7859 -0.0178  0.0013  0.0000
                                          0.5184 -0.0108 -0.3350  0.0133 -0.0001
                                          0.0000  0.0248  0.0104  0.0048
 24. (1.43417) LP ( 2) N  3             s(  0.00%)p 1.00( 99.80%)d 0.00(  0.20%)
                                          0.0000 -0.0001  0.0000  0.9990 -0.0096
                                         -0.0018  0.0000  0.0009  0.0000 -0.0298
                                          0.0332 -0.0001 -0.0001  0.0001
 25. (1.97179) LP ( 1) N  5             s( 70.53%)p 0.42( 29.43%)d 0.00(  0.04%)
                                         -0.0006  0.8396 -0.0215 -0.0007  0.0000
                                          0.0043 -0.0011  0.5421 -0.0200  0.0000
                                          0.0000 -0.0003 -0.0015 -0.0196
 26. (1.84512) LP ( 1) N  6             s( 61.80%)p 0.62( 38.13%)d 0.00(  0.07%)
                                          0.0004  0.7859 -0.0178  0.0013  0.0000
                                          0.5184 -0.0108  0.3350 -0.0133 -0.0001
                                          0.0000 -0.0248  0.0104  0.0048
 27. (1.43416) LP ( 2) N  6             s(  0.00%)p 1.00( 99.80%)d 0.00(  0.20%)
                                          0.0000 -0.0001  0.0000  0.9990 -0.0096
                                         -0.0018  0.0000 -0.0009  0.0000 -0.0298
                                         -0.0332  0.0001 -0.0001  0.0001
 28. (1.97179) LP ( 1) N  8             s( 70.53%)p 0.42( 29.43%)d 0.00(  0.04%)
                                         -0.0006  0.8396 -0.0215 -0.0007  0.0000
                                          0.0043 -0.0011 -0.5421  0.0200  0.0000
```

CCSD/cc-pVDZ

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
N 1	-0.00408	1.99935	4.93386	0.07086	7.00408
N 2	-0.00408	1.99935	4.93386	0.07086	7.00408
N 3	-0.26836	1.99928	5.19904	0.07003	7.26836
N 4	0.24179	1.99921	4.69424	0.06475	6.75821
N 5	0.03064	1.99937	4.90342	0.06656	6.96936
N 6	-0.26836	1.99928	5.19904	0.07003	7.26836
N 7	0.24179	1.99921	4.69424	0.06475	6.75821
N 8	0.03064	1.99937	4.90342	0.06656	6.96936
* Total *	0.00000	15.99444	39.46115	0.54441	56.00000

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.....................................................................
    (Occupancy)   Bond orbital/ Coefficients/ Hybrids
 ---------------------------------------------------------------------------
  1. (1.95741) BD ( 1) N  1- N  2
             ( 50.00%)   0.7071* N  1 s( 32.36%)p 2.08( 67.26%)d 0.01(  0.38%)
                                      -0.0005 -0.5661 -0.0559  0.0000  0.0000
                                      -0.0741  0.0257  0.8153  0.0414  0.0000
                                       0.0000  0.0214  0.0051 -0.0577
             ( 50.00%)   0.7071* N  2 s( 32.36%)p 2.08( 67.26%)d 0.01(  0.38%)
                                      -0.0005 -0.5661 -0.0559  0.0000  0.0000
                                      -0.0741  0.0257 -0.8153 -0.0414  0.0000
                                       0.0000 -0.0214  0.0051 -0.0577
  2. (1.90164) BD ( 2) N  1- N  2
             ( 50.00%)   0.7071* N  1 s(  0.00%)p 1.00( 99.62%)d 0.00(  0.38%)
                                       0.0000  0.0001  0.0000  0.9981  0.0017
                                      -0.0011  0.0000  0.0000  0.0000  0.0227
                                      -0.0575  0.0001  0.0000  0.0000
             ( 50.00%)   0.7071* N  2 s(  0.00%)p 1.00( 99.62%)d 0.00(  0.38%)
                                       0.0000  0.0001  0.0000  0.9981  0.0017
                                      -0.0011  0.0000  0.0000  0.0000  0.0227
                                       0.0575 -0.0001  0.0000  0.0000
  3. (1.89295) BD ( 1) N  1- N  3
             ( 48.50%)   0.6964* N  1 s( 16.52%)p 5.04( 83.18%)d 0.02(  0.30%)
                                       0.0008  0.4060  0.0178  0.0009  0.0000
                                       0.8390 -0.0029  0.3569  0.0212  0.0001
                                       0.0000  0.0205 -0.0477 -0.0183
             ( 51.50%)   0.7176* N  3 s( 16.97%)p 4.87( 82.74%)d 0.02(  0.29%)
                                       0.0000  0.4117  0.0159 -0.0010  0.0000
                                      -0.8224 -0.0049 -0.3882 -0.0194  0.0002
                                       0.0000  0.0126 -0.0474 -0.0211
  4. (1.89295) BD ( 1) N  2- N  6
             ( 48.50%)   0.6964* N  2 s( 16.52%)p 5.04( 83.18%)d 0.02(  0.30%)
                                       0.0008  0.4060  0.0178  0.0009  0.0000
                                       0.8390 -0.0029 -0.3569 -0.0212  0.0001
                                       0.0000 -0.0205 -0.0477 -0.0183
             ( 51.50%)   0.7176* N  6 s( 16.97%)p 4.87( 82.74%)d 0.02(  0.29%)
                                       0.0000  0.4117  0.0159 -0.0011  0.0000
                                      -0.8224 -0.0049  0.3882  0.0194  0.0002
                                       0.0000 -0.0126 -0.0474 -0.0211
  5. (1.95986) BD ( 1) N  3- N  4
             ( 42.09%)   0.6488* N  3 s( 23.15%)p 3.30( 76.46%)d 0.02(  0.39%)
                                       0.0004  0.4776  0.0587 -0.0012  0.0000
                                      -0.1668  0.0195  0.8574  0.0354  0.0001
                                      -0.0002 -0.0301 -0.0089  0.0542
             ( 57.91%)   0.7610* N  4 s( 49.91%)p 1.00( 49.98%)d 0.00(  0.12%)
                                       0.0005  0.7062 -0.0178  0.0012  0.0000
```

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                                      0.0270  0.0145 -0.7063 -0.0017  0.0000
                                     -0.0001 -0.0035 -0.0016  0.0339
 6. (1.89157) BD ( 2) N  3- N  4
            ( 62.29%)   0.7892* N  3 s(  0.00%)p 1.00( 99.71%)d 0.00(  0.29%)
                                      0.0000 -0.0001  0.0000  0.9985  0.0030
                                     -0.0018  0.0000  0.0011  0.0000 -0.0310
                                      0.0440 -0.0001 -0.0002  0.0001
            ( 37.71%)   0.6141* N  4 s(  0.00%)p 1.00( 99.77%)d 0.00(  0.23%)
                                      0.0000 -0.0001  0.0000  0.9988 -0.0119
                                     -0.0018  0.0000  0.0015  0.0000  0.0066
                                     -0.0471  0.0001  0.0001 -0.0001
 7. (1.97141) BD ( 1) N  4- N  5
            ( 56.31%)   0.7504* N  4 s( 49.87%)p 1.00( 50.00%)d 0.00(  0.13%)
                                      0.0004  0.7058  0.0240 -0.0010  0.0000
                                     -0.0317  0.0006  0.7056  0.0342  0.0000
                                     -0.0001  0.0018 -0.0013  0.0366
            ( 43.69%)   0.6610* N  5 s( 31.14%)p 2.20( 68.38%)d 0.02(  0.48%)
                                      0.0005  0.5513  0.0861  0.0010  0.0000
                                     -0.0645 -0.0019 -0.8237 -0.0338  0.0000
                                     -0.0002  0.0060 -0.0002  0.0688
 8. (1.91328) BD ( 2) N  4- N  5
            ( 58.89%)   0.7674* N  4 s(  0.02%)p99.99( 99.81%)d10.89(  0.17%)
                                     -0.0001  0.0035  0.0120  0.0017  0.0000
                                      0.9981 -0.0157  0.0409 -0.0026  0.0000
                                      0.0001  0.0410 -0.0044  0.0011
            ( 41.11%)   0.6412* N  5 s(  0.10%)p99.99( 99.32%)d 5.51(  0.58%)
                                      0.0001  0.0313  0.0080  0.0018  0.0000
                                      0.9948  0.0210 -0.0559 -0.0058  0.0001
                                     -0.0001 -0.0755  0.0015  0.0071
 9. (1.95986) BD ( 1) N  6- N  7
            ( 42.09%)   0.6488* N  6 s( 23.15%)p 3.30( 76.46%)d 0.02(  0.39%)
                                      0.0004  0.4776  0.0587 -0.0011  0.0000
                                     -0.1668  0.0195 -0.8574 -0.0354  0.0001
                                      0.0002  0.0301 -0.0089  0.0542
            ( 57.91%)   0.7610* N  7 s( 49.91%)p 1.00( 49.98%)d 0.00(  0.12%)
                                      0.0005  0.7062 -0.0178  0.0011  0.0000
                                      0.0270  0.0145  0.7063  0.0017  0.0000
                                      0.0001  0.0035 -0.0016  0.0339
10. (1.97141) BD ( 1) N  7- N  8
            ( 56.31%)   0.7504* N  7 s( 49.87%)p 1.00( 50.00%)d 0.00(  0.13%)
                                      0.0004  0.7058  0.0240 -0.0010  0.0000
                                     -0.0317  0.0006 -0.7056 -0.0342  0.0000
                                      0.0001 -0.0018 -0.0013  0.0366
            ( 43.69%)   0.6610* N  8 s( 31.14%)p 2.20( 68.38%)d 0.02(  0.48%)
                                      0.0005  0.5513  0.0861  0.0010  0.0000
                                     -0.0645 -0.0019  0.8237  0.0338  0.0000
                                      0.0002 -0.0060 -0.0002  0.0688
```

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11. (1.93372) BD ( 2) N  7- N  8
            ( 50.46%)   0.7103* N  7 s(  0.00%)p 1.00( 99.75%)d 0.00(  0.25%)
                                      0.0000 -0.0001  0.0000  0.9987 -0.0047
                                     -0.0017  0.0000 -0.0014  0.0000  0.0038
                                     -0.0498  0.0001 -0.0001  0.0001
            ( 49.54%)   0.7039* N  8 s(  0.00%)p 1.00( 99.52%)d 0.00(  0.48%)
                                      0.0000  0.0000  0.0000  0.9976  0.0074
                                     -0.0017  0.0000 -0.0013  0.0000 -0.0016
                                      0.0692 -0.0001  0.0001 -0.0002
12. (1.91328) BD ( 3) N  7- N  8
            ( 58.89%)   0.7674* N  7 s(  0.02%)p99.99( 99.81%)d10.89(  0.17%)
                                     -0.0001  0.0035  0.0120  0.0017  0.0000
                                      0.9981 -0.0157 -0.0409  0.0026  0.0000
                                     -0.0001 -0.0410 -0.0044  0.0011
            ( 41.11%)   0.6412* N  8 s(  0.10%)p99.99( 99.32%)d 5.51(  0.58%)
                                      0.0001  0.0313  0.0080  0.0018  0.0000
                                      0.9948  0.0210  0.0559  0.0058  0.0001
                                      0.0001  0.0755  0.0015  0.0071
13. (1.99934) CR ( 1) N  1           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0006  0.0000  0.0000  0.0000
                                     -0.0008  0.0000  0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
14. (1.99934) CR ( 1) N  2           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0006  0.0000  0.0000  0.0000
                                     -0.0008  0.0000 -0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
15. (1.99929) CR ( 1) N  3           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0004  0.0000  0.0000  0.0000
                                     -0.0001  0.0000 -0.0003  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
16. (1.99921) CR ( 1) N  4           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0006  0.0000  0.0000  0.0000
                                      0.0001  0.0000  0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
17. (1.99937) CR ( 1) N  5           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0001  0.0000  0.0000  0.0000
                                     -0.0001  0.0000  0.0005  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
18. (1.99929) CR ( 1) N  6           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0004  0.0000  0.0000  0.0000
                                     -0.0001  0.0000  0.0003  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
19. (1.99921) CR ( 1) N  7           s(100.00%)p 0.00(  0.00%)
                                      1.0000 -0.0006  0.0000  0.0000  0.0000
                                      0.0001  0.0000 -0.0001  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
20. (1.99937) CR ( 1) N  8           s(100.00%)p 0.00(  0.00%)
```

```
                                          1.0000 -0.0001  0.0000  0.0000  0.0000
                                         -0.0001  0.0000 -0.0005  0.0000  0.0000
                                          0.0000  0.0000  0.0000  0.0000
 21. (1.90548) LP ( 1) N  1               s( 51.33%)p 0.95( 48.61%)d 0.00(  0.06%)
                                          0.0000  0.7160 -0.0267 -0.0006  0.0000
                                         -0.5350  0.0184  0.4462 -0.0213  0.0000
                                          0.0000  0.0215  0.0128 -0.0046
 22. (1.90548) LP ( 1) N  2               s( 51.33%)p 0.95( 48.61%)d 0.00(  0.06%)
                                          0.0000  0.7160 -0.0267 -0.0006  0.0000
                                         -0.5350  0.0184 -0.4462  0.0213  0.0000
                                          0.0000 -0.0215  0.0128 -0.0046
 23. (1.85531) LP ( 1) N  3               s( 60.15%)p 0.66( 39.77%)d 0.00(  0.08%)
                                          0.0003  0.7753 -0.0185  0.0013  0.0000
                                          0.5404 -0.0114 -0.3247  0.0078 -0.0001
                                          0.0001  0.0251  0.0136  0.0027
 24. (1.94517) LP ( 1) N  5               s( 69.34%)p 0.44( 30.61%)d 0.00(  0.05%)
                                         -0.0002  0.8323 -0.0251 -0.0007  0.0000
                                          0.0051 -0.0007  0.5530 -0.0167  0.0000
                                          0.0000 -0.0003 -0.0005 -0.0212
 25. (1.19137) LP ( 2) N  5               s(  0.00%)p 1.00( 99.62%)d 0.00(  0.38%)
                                          0.0000  0.0000  0.0000  0.9980 -0.0149
                                         -0.0017  0.0000  0.0013  0.0000 -0.0016
                                         -0.0615  0.0001  0.0001 -0.0001
 26. (1.85531) LP ( 1) N  6               s( 60.15%)p 0.66( 39.77%)d 0.00(  0.08%)
                                          0.0003  0.7753 -0.0185  0.0013  0.0000
                                          0.5404 -0.0114  0.3247 -0.0078 -0.0001
                                         -0.0001 -0.0251  0.0136  0.0027
 27. (1.47411) LP ( 2) N  6               s(  0.00%)p 1.00( 99.76%)d 0.00(  0.24%)
                                          0.0000 -0.0001  0.0000  0.9987 -0.0134
                                         -0.0018  0.0000 -0.0010  0.0000 -0.0314
                                         -0.0372  0.0001 -0.0002  0.0001
 28. (1.94517) LP ( 1) N  8               s( 69.34%)p 0.44( 30.61%)d 0.00(  0.05%)
                                         -0.0002  0.8323 -0.0251 -0.0007  0.0000
                                          0.0051 -0.0007 -0.5530  0.0167  0.0000
                                          0.0000  0.0003 -0.0005 -0.0212
```

XI. VIBRATIONAL FREQUENCIES

N_8 EEE monomer
PW-PBE-D 60/540 Ry

# mode	[cm-1]	IR
7	65.06	0.0000
8	113.00	0.0000
9	191.35	0.0000
10	201.81	0.0000
11	323.39	0.0000
12	390.84	0.0000
13	448.02	0.0000
14	518.60	0.0000
15	519.06	0.0000
16	648.12	0.0000
17	707.98	0.0000
18	928.64	0.0000
19	1050.69	0.0000
20	1224.89	0.0000
21	1234.16	0.0000
22	1445.70	0.0000
23	2159.43	0.0000
24	2186.17	0.0000

N_8 EEE monomer
PBE-D aug-cc-pVDZ

# mode	[cm-1]	IR
7	57.48	0.121
8	104.75	1.242
9	182.39	0.000
10	182.87	0.000
11	287.86	0.892
12	346.42	37.268
13	386.36	0.000
14	457.46	0.000
15	458.76	3.100
16	608.96	0.000
17	665.18	76.446
18	790.44	92.700
19	921.10	0.000
20	1085.06	478.499
21	1101.23	0.000
22	1355.01	0.000
23	1997.55	1403.930
24	2020.99	0.000

N_8 EEE monomer
wB97X-D aug-cc-pVDZ

# mode	[cm-1]	IR
7	134.79	0.458
8	147.87	3.458
9	235.54	0.000
10	296.92	0.000
11	384.63	1.201
12	429.73	31.206
13	496.08	0.000
14	598.96	8.553
15	601.41	0.012
16	690.82	0.000
17	777.75	19.791
18	1018.68	93.564
19	1164.24	0.000
20	1263.29	49.888
21	1266.53	856.823
22	1650.19	0.000
23	2280.50	1950.338
24	2315.01	0.008

N_8 EZE monomer
PW-PBE-D 60/540 Ry

# mode	[cm-1]	IR
7	82.24	0.0000
8	108.06	0.0000
9	131.31	0.0000
10	225.09	0.0000
11	274.01	0.0000
12	515.07	0.0000
13	540.40	0.0000
14	577.07	0.0000
15	581.32	0.0000
16	605.00	0.0000
17	688.09	0.0000
18	826.10	0.0000
19	905.02	0.0000
20	1223.58	0.0000
21	1232.35	0.0000
22	1490.46	0.0000
23	2151.49	0.0000
24	2181.18	0.0000

N_8 EZE monomer
PBE-D aug-cc-pVDZ

# mode	[cm-1]	IR
7	67.63	0.004
8	97.58	0.012
9	114.12	0.000
10	200.62	10.867
11	248.13	1.229
12	463.84	0.003
13	476.36	9.171
14	486.44	3.826
15	496.18	455.330
16	532.31	0.000
17	574.08	0.657
18	669.15	13.870
19	816.89	274.533
20	1087.40	10.187
21	1107.68	240.127
22	1417.30	58.161
23	1988.56	1508.770
24	2015.00	0.489

N_8 EZE monomer
wB97X-D aug-cc-pVDZ

# mode	[cm-1]	IR
7	81.40	0.159
8	120.57	0.007
9	132.03	0.000
10	234.65	0.438
11	294.65	1.034
12	546.74	0.000
13	561.08	9.062
14	595.27	0.000
15	613.22	0.006
16	636.59	122.296
17	755.76	65.062
18	949.24	19.753
19	1013.27	616.616
20	1253.66	463.845
21	1258.18	12.830
22	1641.95	50.493
23	2277.70	1882.847
24	2308.91	1.185

N_8 solid
PW-PBE-D 60/540 Ry

# mode	[cm-1]	IR
4	35.20	0.0004
5	40.99	0.0114
6	51.98	0.0080
7	64.29	0.0033
8	78.07	0.0039
9	80.36	0.0170
10	97.78	0.0182
11	109.57	0.0019
12	116.22	0.0067
13	128.48	0.0050
14	131.01	0.0031
15	140.96	0.0193
16	145.27	0.0361
17	171.01	0.0025
18	209.00	0.0026
19	222.44	0.0053
20	236.59	0.0516
21	279.04	0.0345
22	327.05	0.0318
23	394.68	0.9072
24	459.38	0.0003
25	508.82	0.0466
26	512.79	0.0330
27	513.25	0.1594
28	534.53	0.2300
29	577.92	0.0435
30	580.52	0.1451
31	604.01	7.4780
32	644.87	0.0555
33	698.83	3.8769
34	709.20	2.6739
35	851.56	0.9760
36	922.56	14.6343
37	944.98	4.0924
38	1074.89	0.0365
39	1219.35	0.8196
40	1225.94	0.8887
41	1230.93	15.5064
42	1254.33	28.0323
43	1430.69	0.0167
44	1482.59	2.2470

45	2151.14	3.9252
46	2169.30	161.1859
47	2179.14	3.6901
48	2194.10	0.0809

XII. CARTESIAN GEOMETRIES AND RELEVANT ENERGIES

N_8 unit cell
PW-PBE-D 60/540 Ry
Final Enthalpy = -450.5651242615 Ry

N	-1.966168820	0.594170583	-0.085877498
N	-3.211947339	0.551190847	0.023842564
N	-3.857165422	0.965504402	-1.152424128
N	-0.831619871	0.578353947	0.007706435
N	-0.630597490	-0.302932637	-3.590605565
N	0.239786222	-0.738016073	-2.601505946
N	-2.330712436	-0.558859227	2.639395138
N	-1.493014347	-0.993393467	3.649366462
N	5.033073798	0.575546316	0.588557852
N	3.785988390	0.633666056	0.549050026
N	2.553445309	-0.469551387	-3.100574298
N	1.428936462	-0.552391152	-2.943289227
N	-3.541200437	-0.755826209	2.877449251
N	-4.677475453	-0.837210835	2.890504880
N	5.607954815	0.965985629	-0.646774824
N	2.653172587	0.630162115	0.674873412

N_8 EEE monomer
PBE-D aug-cc-pVDZ
Enuc: 295.5244229193 hartree
Total Energy: -435.5510337742 hartree

N	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.283946
N	1.393178	0.000000	-0.421351
N	1.453682	0.000000	-1.709771
N	1.736699	0.000000	-2.838803
N	-1.393184	0.000000	1.705279
N	-1.453691	0.000000	2.993701
N	-1.736711	0.000000	4.122731

N_8 EEE monomer
wB97X-D aug-cc-pVDZ
Enuc: 311.1972345685 hartree
Total Energy: -437.6879172650

N	6.164797	-0.307254	0.000000
N	7.124279	0.697270	0.000000
N	4.081885	-0.788695	0.000000
N	5.041679	0.215208	0.000000
N	9.331047	-0.185795	0.000000

N	8.260572	0.164947	0.000000
N	2.945985	-0.254719	0.000000
N	1.876001	0.097266	0.000000

N_8 EZE monomer
PBE-D aug-cc-pVDZ
Enuc: 298.9240022291 hartree
Total Energy: -435.5562314181 hartree

N	0.000208	-0.934334	0.629319
N	0.000208	-0.934334	-0.629319
N	0.001728	0.415463	1.293380
N	-0.000210	0.245884	2.566735
N	-0.001727	0.272988	3.731235
N	0.001728	0.415463	-1.293380
N	-0.000210	0.245884	-2.566735
N	-0.001727	0.272988	-3.731235

N_8 EZE monomer
wB97X-D aug-cc-pVDZ
Enuc: 306.3989829351 hartree
Total Energy: -437.692044885264 hartree

N	-0.304867	2.462267	-0.234802
N	-0.251024	1.215541	-0.376477
N	-0.306668	0.618414	0.894313
N	-0.358784	3.586306	-0.283039
N	-0.251074	-1.215550	-0.376475
N	-0.304871	-2.462280	-0.234797
N	-0.306798	-0.618381	0.894300
N	-0.358751	-3.586321	-0.283024

N_8 codimer
wB97X-D aug-cc-pVDZ
Enuc: 844.3205653363 hartree
Total energy: -875.381137976 hartree

N	1.619983	1.136215	-0.053767
N	0.560618	1.518479	-0.060808
N	2.737140	0.570278	-0.083069
N	3.734308	1.519664	0.217442
N	4.889237	1.079832	0.207594
N	4.998995	-0.281827	-0.109994
N	6.205644	-0.619570	-0.082646
N	7.239148	-1.066656	-0.093179
N	-0.543667	-1.736249	-0.307626

N	-1.633420	-1.659933	-0.028667
N	-2.851332	-1.726386	0.260649
N	-3.381679	-0.436688	0.239501
N	-4.618712	-0.525255	0.196988
N	-5.150397	0.761446	0.215091
N	-6.361900	0.695468	-0.106232
N	-7.443966	0.771182	-0.411275

N_8 EEE dimer

N_8 pentagonal dimer
wB97X-D aug-cc-pVDZ
Enuc: 927.5435347003 hartree
Total Energy: -875.444094803433 hartree

N	-1.463063	1.132130	-2.000000
N	-2.549351	0.410692	-2.000000
N	-0.499138	0.245973	-2.000000
N	-0.926893	-0.996097	-2.000000
N	-2.224091	-0.879021	-2.000000
N	0.816981	0.662594	-2.000000
N	1.584718	-0.335068	-2.000000
N	2.392976	-1.117119	-2.000000
N	6.150566	1.252456	-2.000000
N	5.129469	0.443341	-2.000000
N	7.183380	0.443773	-2.000000
N	6.855071	-0.828373	-2.000000
N	5.554257	-0.816546	-2.000000
N	8.459786	0.965202	-2.000000
N	9.318501	0.046820	-2.000000
N	10.216831	-0.630756	-2.000000

N_4 parallel dimer
wB97X-D aug-cc-pVDZ
Enuc: 329.4698362048 hartree
Total Energy: -437.4648513776 hartree

N	0.505998	-0.843243	1.509358
N	0.923696	0.337459	1.509370
N	-0.923696	-0.337459	1.509370
N	-0.505998	0.843243	1.509357
N	-0.843243	-0.505998	-1.509358
N	0.337459	-0.923696	-1.509370
N	-0.337459	0.923696	-1.509370
N	0.843243	0.505998	-1.509358

N_4 parallel dimer
RI-MOS-MP2 aug-cc-pVDZ
Enuc: 335.9383785026 hartree
Total MP2 Energy: -436.4265033536 hartree

N	-0.340831	-0.956735	1.328404
N	-1.002187	0.164708	1.328404
N	0.340831	0.956735	1.328404
N	1.002187	-0.164708	1.328404
N	-0.956735	0.340831	-1.328404
N	0.164708	1.002187	-1.328404
N	-0.164708	-1.002187	-1.328404
N	0.956735	-0.340831	-1.328404

N_4 tilted dimer
wB97X-D aug-cc-pVDZ
Enuc: 304.5652606525 hartree
Total Energy: -437.465506318127 hartree

N	-1.108745	-0.151973	0.313468
N	-1.943712	-0.975303	-0.117617
N	-2.164680	0.936698	0.291390
N	-3.002616	0.113493	-0.135804
N	1.488445	0.506017	-0.728118
N	2.284871	0.948683	0.127750
N	2.622717	-0.465220	0.550166
N	1.823721	-0.912395	-0.301236

N_4 tilted dimer
RI-MOS-MP2 aug-cc-pVDZ
Enuc: 307.9585007954 hartree
Total Energy: -435.1263892475 hartree

N	-1.069157	0.462611	0.644651
N	-1.952680	1.035726	-0.109895
N	-2.598196	-0.350989	-0.409887
N	-1.718457	-0.930872	0.342748
N	1.071435	-0.470042	-0.642869
N	1.952220	-1.032333	0.123133
N	2.595522	0.357835	0.407980
N	1.719313	0.928066	-0.355861

N_4 tetramer
wB97X-D aug-cc-pVDZ
Enuc: 997.3140442901 hartree

Total Energy: -874.9388548845 hartree

N	1.118570	1.191476	-0.773019
N	1.597037	2.342708	-0.851731
N	0.547264	2.709541	-1.877884
N	0.068675	1.556871	-1.803475
N	-1.402534	1.154393	0.665447
N	-2.559734	1.622644	0.625953
N	-2.992043	0.645248	1.697727
N	-1.835856	0.171620	1.737119
N	-1.197402	-1.424831	-0.708253
N	-1.601912	-2.585677	-0.930237
N	0.049619	-1.702163	-1.524249
N	-0.353218	-2.864373	-1.743657
N	2.736680	-0.841400	0.601575
N	2.942082	-0.223150	1.668212
N	1.546316	-0.567782	2.141140
N	1.336457	-1.185125	1.075332

N_4 tetramer
RI-MOS-MP2 aug-cc-pVDZ
Enuc: 1010.3816776826 hartree
Total MP2 Energy: -872.8657132323 hartree

N	1.312739	0.927030	-0.662574
N	1.993015	2.008682	-0.881829
N	0.948333	2.468415	-1.929834
N	0.255475	1.390890	-1.732455
N	0.932425	-1.224629	1.087213
N	1.015913	-0.619336	2.231681
N	2.548865	-0.477828	2.057547
N	2.490433	-1.079077	0.912105
N	-1.152661	-1.064976	-0.833472
N	-1.719776	-2.204453	-1.080558
N	-0.471643	-2.670306	-1.870440
N	0.116488	-1.539855	-1.636509
N	-1.870270	0.130111	1.545370
N	-2.986179	0.776612	1.416482
N	-2.272849	1.899935	0.632918
N	-1.140308	1.278787	0.744357