Experimental and computational evidence for 'double pancake bonds'; the role of dispersion-corrected DFT methods in strongly dimerized 5-aryl-1λ²,3λ²-dithia-2,4,6-triazines

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SUPPORTING MATERIAL

1) Full Crystallographic Data for 3 and 4............................................................... S2
   Table S1 Crystal, Data Collection and Refinement Parameters for Crystallography of 3 and 4..... S2
   Table S2. Fractional Atomic Coordinates for 3 ......................................................... S3
   Table S3. Bond lengths [Å] and angles [*] for 3..................................................... S4
   Table S4. Torsion angles [*] for 3........................................................................ S5
   Table S5. Atomic Occupancy for 3....................................................................... S6
   Table S6 Fractional Atomic Coordinates for 4......................................................... S6
   Table S7. Bond lengths [Å] and angles [*] for 4..................................................... S6
   Table S8. Torsion angles [*] for 4........................................................................ S7
   Table S9 Least Squares Planes in crystal structure of 3............................................ S8
   Figure S1 Full view of a displacement ellipsoids plot of 3........................................ S9
   Figure S2 View of the molecular structure of the dimer 3 orthogonal to the aryl planes........ S10
   Figure S3 Packing diagrams showing intermolecular contacts in the lattice of 3 at 100 K........ S11
   Figure S4 Packing diagram for (a) 1 (refcode: DESSID) and (b) 2 (refcode: PAFLAJ) ........ S12
   Figure S5 Diagram for the crystal structure of 4 showing contacts and packing diagram .... S13
   Table S10. Selected geometrical parameters from experiments and DFT calculations........ S14

2) DFT Computational Results.................................................................................. S15
   Table S11 DFT Computed Results for the ‘parent’ HCN₃S₂ dimer................................. S17
   Table S12 DFT Computed Results for the CF₃CN₃S₂ dimer......................................... S17
   Table S13 DFT Computed Results for the Me₂NCN₃S₂ dimer.................................... S17
   Table S14 DFT Computed Cartesian Geometries with Structure Plots ..................... S18

(39 Pages)
Table S1. Crystal, Data Collection and Refinement Parameters for Crystallography of 3 and 4

| Parameter                        | 3       | 3-CF₃-C₆H₄-CN₃S₂ | 4       | 3-CF₃-C₆H₄-CN₃S₃ |
|----------------------------------|---------|------------------|---------|------------------|
| Identification code              | RB16082 |                  | RB16083rf1 |                   |
| Empirical formula                | C₈H₄F₃N₃S₂  |                | C₈H₄F₃N₃S₃  |                   |
| Formula weight                   | 263.26  |                  | 323.34  |                  |
| Temperature/K                    | 99.98(13) |                | 100.01(10) |                 |
| Crystal system                   | triclinic |                | monoclinic |                 |
| Space group                      | P-1     |                  | C2/c    |                  |
| a/Å                              | 7.62509(11) |              | 22.90772(16) |            |
| b/Å                              | 8.44847(12) |              | 4.66989(3)  |                  |
| c/Å                              | 15.92585(16) |          | 22.2724(2)  |                  |
| α/°                              | 104.2308(10) |             | 90      |                  |
| β/°                              | 94.4500(10)  |              | 106.6781(9) |                  |
| γ/°                              | 103.1503(12) |            | 90      |                  |
| Volume/Å³                        | 958.65(2)  |              | 2282.39(3) |                  |
| Z                                | 4        |                  | 8       |                  |
| ρcalc/g/cm³                      | 1.824    |                  | 1.882   |                  |
| μ/mm⁻¹                           | 5.289    |                  | 6.306   |                  |
| F(000)                           | 528.0    |                  | 1296.0  |                  |
| Crystal size/mm³                 | 0.374 × 0.25 × 0.061 |         | 0.385 × 0.25 × 0.063 | |
| Radiation                        | CuKα (λ = 1.54184) |         | CuKα (λ = 1.54184) |       |
| 2θ range for data collection/°   | 11.102 to 154.986 |        | 8.058 to 155.214 |       |
| Index ranges                     | -9 ≤ h ≤ 9, -10 ≤ k ≤ 10, -20 ≤ l ≤ 20 |       | -28 ≤ h ≤ 28, -5 ≤ k ≤ 5, -27 ≤ l ≤ 27 | |
| Reflections collected            | 37748    |                  | 23650   |                  |
| Independent reflections          | 4013 [Rint = 0.0533, Rsigma = 0.0198] |      | 2390 [Rint = 0.0276, Rsigma = 0.0108] | |
| Data/restraints/parameters       | 4013/30/320 |                | 2390/0/172 |                 |
| Goodness-of-fit on F²            | 1.082    |                  | 1.075   |                  |
| Final R indexes [I>2σ (I)]      | R₁ = 0.0385, wR₂ = 0.1067 |        | R₁ = 0.0280, wR₂ = 0.0741 |       |
| Final R indexes [all data]      | R₁ = 0.0398, wR₂ = 0.1076 |        | R₁ = 0.0286, wR₂ = 0.0744 |       |
| Largest diff. peak/hole / e Å⁻³  | 0.51/-0.48 |              | 0.41/-0.32 |               |

A = 1/[σ²(Fo²) + A(P)² + BP] where P = (Fo² + 2Fc²)/3.
Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2\times 10^3$) for 3. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$ tensor.

| Atom | x        | y        | z        | $U(eq)$  |
|------|----------|----------|----------|----------|
| S1   | 9440.8(6)| 10155.4(6)| 1261.4(3)| 18.58(13)|
| S2   | 6016.5(6)| 8369.4(6)| 336.9(3) | 17.89(13)|
| S3   | 7338.0(6)| 5966.8(6)| -322.2(3)| 16.75(13)|
| S4   | 10752.8(6)| 7757.9(6)| 610.9(3) | 17.64(13)|
| F1   | 10343.5(19)| 7494(2)  | 4558.2(9)| 40.8(4)  |
| F2   | 8921.4(19)| 8658.1(19)| 5543.0(8)| 36.2(3)  |
| F3   | 8246(2)  | 5959.5(19)| 5057.2(10)| 16.7(3)  |
| N1   | 8654(2)  | 9403(2)  | 2026.0(10)| 18.2(3)  |
| N2   | 7890(2)  | 9831(2)  | 428.0(11) | 20.2(3)  |
| N3   | 5665(2)  | 7884(2)  | 1235.8(11)| 19.1(3)  |
| N4   | 7164(2)  | 5105(2)  | 475.4(10) | 17.0(3)  |
| N5   | 9364(2)  | 7109(2)  | -310.7(11)| 19.3(3)  |
| N6   | 10139(2) | 6662(2)  | 1280.5(11)| 18.4(3)  |
| C1   | 6956(3)  | 8422(2)  | 1935.8(12)| 18.1(4)  |
| C2   | 6430(3)  | 7936(2)  | 2734.4(12)| 18.4(4)  |
| C3   | 7781(3)  | 7939(2)  | 3380.4(13)| 19.9(4)  |
| C4   | 7288(3)  | 7456(3)  | 4119.5(13)| 22.2(4)  |
| C5   | 5462(3)  | 7019(3)  | 4234.6(14)| 25.8(4)  |
| C6   | 4134(3)  | 7039(3)  | 3596.8(14)| 26.7(4)  |
| C7   | 4604(3)  | 7473(3)  | 2841.4(13)| 21.9(4)  |
| C8   | 8697(3)  | 7397(3)  | 4810.0(13)| 26.7(4)  |
| C11  | 8515(3)  | 5535(2)  | 1151.1(12)| 16.5(4)  |
| C12  | 8200(3)  | 4599(2)  | 1820.5(12)| 16.7(4)  |
| C13  | 6446(3)  | 3834(2)  | 1923.1(12)| 18.3(4)  |
| C14  | 6166(3)  | 2994(2)  | 2568.0(12)| 18.5(4)  |
| C15  | 7627(3)  | 2897(2)  | 3116.8(12)| 20.4(4)  |
| C16  | 9386(3)  | 3654(3)  | 3010.6(13)| 21.4(4)  |
| C17  | 9675(3)  | 4502(2)  | 2368.1(12)| 18.7(4)  |
| F4   | 4134(18) | 1750(30) | 3420(9)  | 51(2)    |
| F5   | 3650(20) | 601(19)  | 2056(8)  | 36(2)    |
| F6   | 3110(20) | 3030(20) | 2512(16) | 43(3)    |
| C18  | 4260(120)| 2160(110)| 2660(60) | 24.2(4)  |
| F4A  | 4000(20) | 2360(60) | 3477(9)  | 59(5)    |
| F5A  | 3750(30) | 610(30)  | 2230(30) | 59(4)    |
| F6A  | 3000(30) | 2870(30) | 2370(20) | 38(3)    |
| C18A | 4260(170)| 2160(160)| 2660(80) | 24.2(4)  |
Table S3. Bond lengths [Å] and angles [°] for 3

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|------|------|----------|------|------|----------|
| S1   | S4   | 2.4956(6) | C3   | C4   | 1.389(3) |
| S1   | N1   | 1.6024(16) | C4   | C5   | 1.396(3) |
| S1   | N2   | 1.6328(17) | C4   | C8   | 1.494(3) |
| S2   | S3   | 2.5069(6)  | C5   | C6   | 1.384(3) |
| S2   | N2   | 1.6320(17) | C6   | C7   | 1.391(3) |
| S2   | N3   | 1.6087(17) | C11  | C12  | 1.479(3) |
| S3   | N4   | 1.6117(16) | C12  | C13  | 1.388(3) |
| S3   | N5   | 1.6209(17) | C12  | C17  | 1.399(3) |
| S4   | N5   | 1.6355(17) | C13  | C14  | 1.388(3) |
| S4   | N6   | 1.6058(16) | C14  | C15  | 1.392(3) |
| F1   | C8   | 1.339(3)   | C14  | C18  | 1.50(9)  |
| F2   | C8   | 1.342(2)   | C14  | C18A | 1.50(12) |
| F3   | C8   | 1.347(3)   | C15  | C16  | 1.391(3) |
| N1   | C1   | 1.344(3)   | C16  | C17  | 1.390(3) |
| N3   | C1   | 1.340(3)   | F4   | C18  | 1.34(10) |
| N4   | C11  | 1.348(2)   | F5   | C18  | 1.38(8)  |
| N6   | C11  | 1.345(3)   | F6   | C18  | 1.31(11) |
| C1   | C2   | 1.486(3)   | F4A  | C18A | 1.31(13) |
| C2   | C3   | 1.398(3)   | F5A  | C18A | 1.27(12) |
| C2   | C7   | 1.394(3)   | F6A  | C18A | 1.36(15) |

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|------|------|------|---------|------|------|------|---------|
| N1   | S1   | S4   | 95.79(6) | F1   | C8   | F3   | 106.52(19) |
| N1   | S1   | N2   | 112.87(9)| F1   | C8   | C4   | 113.47(17) |
| N2   | S1   | S4   | 96.47(6) | F2   | C8   | F3   | 105.77(17) |
| N2   | S2   | S3   | 94.87(6) | F2   | C8   | C4   | 112.60(18) |
| N3   | S2   | S3   | 97.05(6) | F3   | C8   | C4   | 111.76(18) |
| N3   | S2   | N2   | 113.54(9)| N4   | C11  | C12  | 115.77(16) |
| N4   | S3   | S2   | 96.42(6) | N6   | C11  | N4   | 128.46(17) |
| N4   | S3   | N5   | 113.69(9)| N6   | C11  | C12  | 115.73(16) |
| N5   | S3   | S2   | 96.41(6) | C13  | C12  | C11  | 120.60(17) |
| N5   | S4   | S1   | 95.16(6) | C13  | C12  | C17  | 119.32(17) |
| N6   | S4   | S1   | 96.77(6) | C17  | C12  | C11  | 120.07(17) |
| N6   | S4   | N5   | 112.37(9)| C12  | C13  | C14  | 120.05(17) |
| C1   | N1   | S1   | 122.87(14)| C13  | C14  | C15  | 120.95(18) |
| S2   | N2   | S1   | 117.39(10)| C13  | C14  | C18  | 119(4) |
| C1   | N3   | S2   | 121.67(14)| C13  | C14  | C18A | 119(5) |
| C11  | N4   | S3   | 121.53(14)| C15  | C14  | C18  | 120(4) |
| S3   | N5   | S4   | 117.85(10)| C15  | C14  | C18A | 120(5) |
| C11  | N6   | S4   | 123.00(14)| C16  | C15  | C14  | 119.00(18) |
| N1   | C1   | C2   | 115.12(17)| C17  | C16  | C15  | 120.35(18) |
| N3   | C1   | N1   | 128.68(18)| C16  | C17  | C12  | 120.32(18) |
| N3   | C1   | C2   | 116.15(17)| F4   | C18  | C14  | 113(6) |
| C3   | C2   | C1   | 119.55(17)| F4   | C18  | F5   | 102(6) |
| C7   | C2   | C1   | 120.53(17)| F5   | C18  | C14  | 111(6) |
| C7   | C2   | C3   | 119.92(18)| F6   | C18  | C14  | 112(7) |
C4  C3  C2  119.55(18)  F6  C18  F4  112(7)
C3  C4  C5  120.59(19)  F6  C18  F5  106(6)
C3  C4  C8  120.89(19)  F4A  C18A  C14  112(7)
C5  C4  C8  118.51(18)  F4A  C18A  F6A  100(9)
C6  C5  C4  119.48(19)  F5A  C18A  C14  114(10)
C5  C6  C7  120.55(19)  F5A  C18A  F4A  111(10)
C6  C7  C2  119.87(19)  F5A  C18A  F6A  105(8)
F1  C8  F2  106.16(18)  F6A  C18A  C14  114(10)

### Table S4. Torsion angles [°] for 3

| A  | B  | C  | D  | Angle/°  | A  | B  | C  | D  | Angle/°  |
|----|----|----|----|----------|----|----|----|----|----------|
| S1 | S4 | N5 | S3 | -80.11(10) | C3 | C2 | C7 | C6 | 0.9(3)   |
| S1 | S4 | N6 | C11| 88.04(15)  | C3 | C4 | C5 | C6 | 1.2(3)   |
| S1 | N1 | C1 | N3 | 1.1(3)     | C3 | C4 | C8 | F1 | -13.2(3) |
| S1 | N1 | C1 | C2 | -176.19(13)| C3 | C4 | C8 | F2 | 107.4(2) |
| S2 | S3 | N4 | C11| -89.93(14) | C3 | C4 | C8 | F3 | -133.7(2)|
| S2 | S3 | N5 | S4 | 80.55(10)  | C4 | C5 | C6 | C7 | 0.7(3)   |
| S2 | N3 | C1 | N1 | 0.6(3)     | C5 | C4 | C8 | F1 | 167.0(2) |
| S2 | N3 | C1 | C2 | 177.80(13) | C5 | C4 | C8 | F2 | -72.4(3) |
| S3 | S2 | N2 | S1 | -80.28(10) | C5 | C4 | C8 | F3 | 46.5(3)  |
| S3 | S2 | N3 | C1 | 87.33(15)  | C5 | C6 | C7 | C2 | -1.7(3)  |
| S3 | N4 | C11| N6 | -0.4(3)    | C7 | C2 | C3 | C4 | 0.9(3)   |
| S3 | N4 | C11| C12| -177.79(12)| C8 | C4 | C5 | C6 | -179.0(2)|
| S4 | S1 | N1 | C1 | -91.41(15) | C11| C12| C13| C14| -178.41(16)|
| S4 | S1 | N2 | S2 | 80.93(10)  | C11| C12| C17| C16| 178.63(17)|
| S4 | N6 | C11| N4 | 0.8(3)     | C12| C13| C14| C15| -0.3(3)  |
| S4 | N6 | C11| C12| 178.13(13) | C12| C13| C14| C18| -179(4)  |
| N1 | S1 | N2 | S2 | -18.16(14) | C12| C13| C14| C18A| -179(5) |
| N1 | C1 | C2 | C3 | -23.4(2)   | C13| C12| C17| C16| -0.3(3)  |
| N1 | C1 | C2 | C7 | 156.78(18) | C13| C14| C15| C16| -0.1(3)  |
| N2 | S1 | N1 | C1 | 8.12(18)   | C13| C14| C18| F4 | -165(4)  |
| N2 | S2 | N3 | C1 | -11.14(18) | C13| C14| C18| F5 | 81(7)    |
| N3 | S2 | N2 | S1 | 19.60(14)  | C13| C14| C18| F6 | -37(7)   |
| N3 | C1 | C2 | C3 | 158.95(17) | C13| C14| C18A| F4A| -140(8) |
| N3 | C1 | C2 | C7 | -20.8(3)   | C13| C14| C18A| F5A| 93(10)   |
| N4 | S3 | N5 | S4 | -19.37(14) | C13| C14| C18A| F6A| -27(10) |
| N4 | C11| C12| C13| -23.1(2)   | C14| C15| C16| C17| 0.3(3)   |
| N4 | C11| C12| C17| 158.05(17) | C15| C14| C18| F4 | 17(8)    |
| N5 | S3 | N4 | C11| 9.98(18)   | C15| C14| C18| F5 | -98(6)   |
| N5 | S4 | N6 | C11| -10.40(18) | C15| C14| C18| F6 | 144(4)   |
| N6 | S4 | N5 | S3 | 19.40(14)  | C15| C14| C18A| F4A| 42(12)   |
| N6 | C11| C12| C13| 159.22(17) | C15| C14| C18A| F5A| -86(10)  |
| N6 | C11| C12| C17| -19.7(2)   | C15| C14| C18A| F6A| 155(5)   |
| C1 | C2 | C3 | C4 | -178.88(17)| C15| C16| C17| C12| -0.1(3)  |
| C1 | C2 | C7 | C6 | -179.27(18)| C17| C12| C13| C14| 0.5(3)   |
| C2 | C3 | C4 | C5 | -2.0(3)    | C18| C14| C15| C16| 179(4)   |
| C2 | C3 | C4 | C8 | 178.22(18) | C18A| C14| C15| C16| 179(5)   |
Table S5. Atomic Occupancy for 3

| Atom | Occupancy | Atom | Occupancy | Atom | Occupancy |
|------|-----------|------|-----------|------|-----------|
| F4   | 0.58(7)   | F5   | 0.58(7)   | F6   | 0.58(7)   |
| C18  | 0.58(7)   | F4A  | 0.42(7)   | F5A  | 0.42(7)   |
| F6A  | 0.42(7)   | C18A | 0.42(7)   |

Table S6 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 4. \(U_{eq}\) is defined as 1/3 of the trace of the orthogonalised \(U_{ij}\) tensor.

| Atom | \(x\)    | \(y\)    | \(z\)    | \(U_{eq}\) |
|------|----------|----------|----------|------------|
| S2   | 3381.3(2)| 2542.9(8)| 5493.1(2)| 16.45(11)  |
| S1   | 4513.2(2)| 2553.7(8)| 5342.2(2)| 14.68(11)  |
| S3   | 4317.9(2)| 5637.3(8)| 6372.4(2)| 16.41(11)  |
| F1   | 4570.7(5)| 9676(3)  | 3021.8(5)| 32.3(3)    |
| F2   | 4047.2(5)| 13499(2)| 2725.9(5)| 28.6(2)    |
| F3   | 3780.5(5)| 9586(2)  | 2219.8(5)| 29.7(3)    |
| N2   | 3976.2(6)| 636(3)   | 5489.5(6)| 17.8(3)    |
| N1   | 4228.7(6)| 4760(3)  | 4772.6(6)| 16.6(3)    |
| N3   | 3210.7(6)| 4735(3)  | 4905.3(6)| 17.6(3)    |
| N5   | 3634.4(6)| 4840(3)  | 6132.7(6)| 18.6(3)    |
| N5   | 4757.2(6)| 4839(3)  | 5984.9(6)| 17.1(3)    |
| C1   | 3636.6(7)| 5475(3)  | 4630.8(7)| 14.4(3)    |
| C2   | 3418.5(7)| 7392(3)  | 4075.5(7)| 14.6(3)    |
| C3   | 3802.7(7)| 8058(3)  | 3707.9(7)| 15.2(3)    |
| C4   | 3604.8(7)| 9942(3)  | 3211.1(7)| 15.9(3)    |
| C5   | 3026.0(7)| 11180(4)| 3070.4(7)| 19.1(3)    |
| C6   | 2641.9(7)| 10476(4)| 3429.7(8)| 20.3(3)    |
| C7   | 2834.8(7)| 8591(4)  | 3928.1(7)| 18.0(3)    |
| C8   | 4001.7(7)| 10672(3)| 2800.7(7)| 17.9(3)    |

Table S7. Bond lengths [Å] and angles [°] for 4

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|------|------|----------|------|------|----------|
| S2   | N2   | 1.6296(13)| N1   | C1   | 1.3436(19) |
| S2   | N3   | 1.6190(14)| N3   | C1   | 1.337(2)   |
| S2   | N5   | 1.7440(15)| C1   | C2   | 1.492(2)   |
| S1   | N2   | 1.6292(13)| C2   | C3   | 1.398(2)   |
| S1   | N1   | 1.6192(13)| C2   | C7   | 1.399(2)   |
| S1   | N4   | 1.7437(14)| C3   | C4   | 1.384(2)   |
| S3   | N5   | 1.5478(14)| C4   | C5   | 1.397(2)   |
| S3   | N4   | 1.5475(13)| C4   | C8   | 1.502(2)   |
| F1   | C8   | 1.3376(19)| C5   | C6   | 1.388(2)   |
| F2   | C8   | 1.3388(19)| C6   | C7   | 1.386(2)   |
| F3   | C8   | 1.3460(18)|      |      |           |

continued...
### Table S8. Torsion angles [°] for 3

| A    | B    | C    | D    | Angle/° | A    | B    | C    | D    | Angle/° |
|------|------|------|------|---------|------|------|------|------|---------|
| N2   | S2   | N5   |      | 104.93(7) | C3   | C2   | C7   |      | 119.56(14) |
| N3   | S2   | N2   |      | 110.47(7) | C7   | C2   | C1   |      | 120.31(14) |
| N3   | S2   | N5   |      | 102.60(7) | C4   | C3   | C2   |      | 119.52(14) |
| N2   | S1   | N4   |      | 104.70(7) | C3   | C4   | C5   |      | 120.95(14) |
| N1   | S1   | N2   |      | 110.49(7) | C3   | C4   | C8   |      | 120.94(14) |
| N1   | S1   | N4   |      | 102.46(7) | C5   | C4   | C8   |      | 118.10(14) |
| N4   | S3   | N5   |      | 120.33(8) | C6   | C5   | C4   |      | 119.37(15) |
| S1   | N2   | S2   |      | 112.43(8) | C7   | C6   | C5   |      | 120.20(15) |
| C1   | N1   | S1   |      | 119.64(11)| C6   | C7   | C2   |      | 120.38(14) |
| C1   | N3   | S2   |      | 119.65(11)| F1   | C8   | F2   |      | 106.64(13) |
| S3   | N5   | S2   |      | 119.73(8) | F1   | C8   | F3   |      | 106.33(13) |
| S3   | N4   | S1   |      | 119.92(8) | F1   | C8   | C4   |      | 113.16(13) |
| N1   | C1   | C2   |      | 114.78(13)| F2   | C8   | F3   |      | 105.84(13) |
| N3   | C1   | N1   |      | 130.41(14)| F2   | C8   | C4   |      | 112.45(13) |
| N3   | C1   | C2   |      | 114.80(13)| F3   | C8   | C4   |      | 111.90(13) |
| C3   | C2   | C1   |      | 120.11(13)|      |      |      |      |         |
Table S9 Least Squares Planes in crystal structure of 3

Least-squares planes (x, y, z in crystal coordinates) and deviations from them in the crystal structure refinement of 3 (* indicates atom used to define plane)

-4.3989 (0.0026) x + 7.2842 (0.0024) y + 2.4007 (0.0089) z = 3.5387 (0.0034)
  * 0.0010 (0.0012) C1
  * -0.0103 (0.0010) N1
  * 0.0088 (0.0010) N3
  * 0.0085 (0.0006) S1
  * -0.0081 (0.0006) S2
  0.2546 (0.0018) N2
Rms deviation of fitted atoms = 0.0080

-4.8166 (0.0017) x + 5.7526 (0.0118) y + 6.7269 (0.0268) z = 2.1433 (0.0098)
Angle to previous plane (with approximate esd) = 17.457 (0.152)
  * 0.0000 (0.0000) S1
  * 0.0000 (0.0000) N2
  * 0.0000 (0.0000) S2
Rms deviation of fitted atoms = 0.0000

-4.7807 (0.0024) x + 6.1866 (0.0032) y + 5.6562 (0.0083) z = 0.0023 (0.0035)
Angle to previous plane (with approximate esd) = 4.399 (0.181)
  * 0.0026 (0.0012) C11
  * 0.0002 (0.0009) N4
  * -0.0037 (0.0010) N6
  * -0.0012 (0.0006) S3
  * 0.0022 (0.0006) S4
  -0.2567 (0.0018) N5
Rms deviation of fitted atoms = 0.0023

1.9732 (0.0084) x + 3.1878 (0.0019) y + 14.9317 (0.0078) z = 9.4804 (0.0047)
  * -0.1027 (0.0007) C1
  * -0.0021 (0.0009) N1
  * -0.2961 (0.0007) N2
  * 0.2012 (0.0006) S1
  * 0.1996 (0.0006) S2
  -0.2961 (0.0007) N2
Rms deviation of fitted atoms = 0.1890

2.6746 (0.0045) x + 0.7967 (0.0070) y + 20.1283 (0.0056) z = 12.1636 (0.0085)
Angle to previous plane (with approximate esd) = 17.822 (0.140)
  * 0.0000 (0.0000) S3
  * 0.0000 (0.0000) N5
  * 0.0000 (0.0000) S4
Rms deviation of fitted atoms = 0.0000

Least-squares planes (x, y, z in crystal coordinates) and deviations from them in the crystal structure refinement of 4 (* indicates atom used to define plane)

1.9732 (0.0084) x + 3.1878 (0.0019) y + 14.9317 (0.0078) z = 9.4804 (0.0047)
  * -0.1027 (0.0007) C1
  * -0.0021 (0.0009) N1
  * -0.2961 (0.0007) N2
  * 0.2012 (0.0006) S1
  * 0.1996 (0.0006) S2
  -0.2961 (0.0007) N2
Rms deviation of fitted atoms = 0.1890

2.6746 (0.0045) x + 0.7967 (0.0070) y + 20.1283 (0.0056) z = 12.1636 (0.0085)
Angle to previous plane (with approximate esd) = 33.227 (0.098)
  * 0.0000 (0.0000) S1
  * 0.0000 (0.0000) S2
  * 0.0000 (0.0000) N2
Rms deviation of fitted atoms = 0.0000

1.6105 (0.0082) x - 3.7723 (0.0007) y + 12.0374 (0.0078) z = 6.1836 (0.0031)
Angle to previous plane (with approximate esd) = 63.704 ( 0.078 )
* 0.0106 (0.0005) S1
* -0.0385 (0.0007) N4
* 0.0559 (0.0007) S3
* -0.0419 (0.0007) N5
* 0.0139 (0.0005) S2
Rms deviation of fitted atoms = 0.0365
1.9732 (0.0084) x + 3.1878 (0.0019) y + 14.9317 (0.0078) z = 9.4804 (0.0047)

Angle to previous plane (with approximate esd) = 83.069 ( 0.026 )
* -0.1027 (0.0007) C1
* -0.0021 (0.0009) N1
* -0.2961 (0.0007) N2
* 0.2012 (0.0007) S1
* 0.1996 (0.0006) S2
-0.2961 (0.0007) N2
Rms deviation of fitted atoms = 0.1890
2.6746 (0.0045) x + 0.7967 (0.0070) y + 20.1283 (0.0056) z = 12.1636 (0.0017)

Angle to previous plane (with approximate esd) = 33.227 ( 0.098 )
* 0.0000 (0.0000) S1
* 0.0000 (0.0000) S2
* 0.0000 (0.0000) N2
Rms deviation of fitted atoms = 0.0000

Figure S1  Full view of a displacement ellipsoids plot of 3 as found in the crystal lattice and showing the disorder model for the C18 CF₃ group (refined to an occupancy ratio of 0.58:0.42).
Figure S2  View of the molecular structure of the dimer 3 orthogonal to the plane defined by the C12 > C17 phenyl ring (H-atoms omitted). The upper C2 > C7 ring is displaced towards optimal π-stacking with the ring centroid centred over the C13-C14 bond of the lower ring. Some inter-annular C-C distances are shown.
Figure S3  Packing diagrams showing intermolecular contacts in the lattice of 3 at 100 K. (a) Paradigmatic approximately parallel S⋯N contacts link two dimers centrosymmetrically at 3.073 and 2.987 Å are 0.28 and 0.36 Å less than the sums of the v.d.Waals radii, respectively. Symmetry code i: 2-x,2-y,-z. (b) xtended short contacts up to 0.1 Å less than the sums of v.d.Waals radii of the interacting atoms. The pairs of dimers shown in Fig. 3 are further connected by contacts between the apical N atoms and the ring C atoms to form walls of DTTA dimers. Cross-links between these walls have the [CN$_3$S$_2$] units off-register by half resulting in rather long contacts; the metrically shortest contacts are consequently between ortho H atoms of the phenyl ring and sulfur and F to S contacts.

Lattice interactions in the structure of 3

Discuss the short contacts in the crystal. Strongly-associated dimers of dimers. Extended network of contacts less than the sums of the v.d.Waals radii form into parallel 'walls' of dimers that are out of register by half the vertical distance. This long-range organization of the crystal lattice found in 3 is contrasted with that in the only other structurally characterized DTTAs, 1 and 2 (refcodes: DESSID and PAFLAJ), in Fig. S3. 1 shows a layer structure of weakly-associated dimers oriented along the cell b axis, resulting in columns of CN$_3$S$_2$ rings isolated by phenyl rings. The extended structure of 2 shares many similarities with that of 1 and both are significantly different from the more complex pattern of interactions found in 3.
Figure S4 Packing diagram for (a) 1 (refcode: DESSID) and (b) 2 (refcode: PAFLAJ). Contacts between S atoms are colour-coded by length (yellow – very short; purple very long).

Lattice interactions in the structure of 4

The shortest contacts in the crystal lattice are those that connect S3 on one molecule with the N2 of the next molecule which are shorter than (Σrdw=0.30 Å). This leads to 'nesting' of one cage with the next above and below it in an infinite row or 'stack'. At (Σrdw=0.20 Å) the nesting is augmented by an N1 to C1 contact. The stacks of nested cages are aligned with the crystallographic b axis (see Fig. S5). At (Σrdw=0.20 Å) additional short contacts link the rows of nested cages with a second row via centrosymmetric S1···S1" and N1···N1" contacts, so that within the C2/c unit cells, there are four such "pairs" of cages grouped around 1̅ locations.
Figure S5  Diagram for the crystal structure of 4 showing (a) the rows formed by 'nesting' the cages within themselves through short N2⋯S3' and N2⋯C1' contacts and the centrosymmetrically disposed second row of nested cages connected through S1⋯S1'' and N1⋯N1'' contacts. The double-nested rows run along the crystallographic b axis in perfect stacks. (b) Packing diagram viewed down the crystallographic b axis.

Nesting is also observed in structures with CSD Refcodes: AJIHAC (4-NCC6H4), DOSBAO (iPr2N, but very long and weak contacts); ECEBOE (CF3); GEDHEC (Cl-); JAIXOH (CF3). The remaining 11 structures in the literature instead show a head-to-head packing arrangement of N2⋯S3' and S3⋯N2' (refcodes: AJIGAB, AJIGEF, AJIGIJ, AJIGOP, AJIGUV, BEZRUU, BEZSAB, BEZSEF, BEZSIJ, BEZSOP, DACDEQ).
Table S10. Selected geometrical parameters from experiments and DFT calculations.

| Atoms       | 3 b  | 3a b | 3b  | 3c  | 3d' | 3e  | 3f  |
|-------------|------|------|------|------|------|------|------|
| S1–N1       | 1.6024(16) | 1.6130 | 1.615 | 1.643 | 1.616 | 1.620 | 1.675 |
| S3–N4       | 1.6117(16) | 1.6130 | 1.614 | 1.616 | 1.616 | 1.620 | 1.626 |
| S1–N2       | 1.6328(17) | 1.6486 | 1.651 | 1.719 | 1.623 | 1.649 | 1.768 |
| S3–N5       | 1.6209(17) | 1.6487 | 1.652 | 1.635 | 1.623 | 1.648 | 1.639 |
| S2–N2       | 1.6320(17) | 1.6332 | 1.631 | 1.677 | 1.620 | 1.649 | 1.750 |
| S4–N5       | 1.6355(17) | 1.6332 | 1.630 | 1.635 | 1.620 | 1.649 | 1.643 |
| S2–N3       | 1.6087(17) | 1.6111 | 1.610 | 1.623 | 1.659 | 1.620 | 1.568 |
| S4–N6       | 1.6058(16) | 1.6112 | 1.611 | 1.611 | 1.659 | 1.620 | 1.628 |
| N1–C1       | 1.344(3)  | 1.3386 | 1.338 | 1.356 | 1.364 | 1.339 | 1.305 |
| N4–C11      | 1.348(2)  | 1.3379 | 1.338 | 1.345 | 1.364 | 1.339 | 1.337 |
| N3–C1       | 1.340(3)  | 1.3379 | 1.338 | 1.316 | 1.313 | 1.339 | 1.369 |
| N6–C11      | 1.345(3)  | 1.3386 | 1.338 | 1.328 | 1.313 | 1.339 | 1.336 |
| C1–C2       | 1.486(3)  | 1.4790 | 1.479 | 1.482 | 1.481 | 1.438 | 1.481 |
| C11–C12     | 1.479(3)  | 1.4790 | 1.480 | 1.479 | 1.481 | 1.438 | 1.483 |
| S1…S4       | 2.4956(6) | 2.5496 | 2.549 | 2.0753 a | 2.6971 | 2.4649 | 1.8155 b |
| S2…S3       | 2.5069(6) | 2.5496 | 2.550 | —    | —    | 2.4650 | 2.5244 |
| i – i'      | 2.759    | 2.798  | 2.796 | 2.665 | 2.775 | 3.226 | 3.472 |
| ii – ii'    | 3.850    | 3.570  | 3.633 | —    | —    | —    | —    |

| Tip angle S1N2S2 | 17.46(15) | 17.96 | 17.93 | 16.40 | 8.52 | 30.21 | 54.22 |
| Tip angle S3N5S4 | 17.82(14) | 17.96 | 17.95 | 36.77 | 8.52 | 30.21 | 42.71 |

a This value S1…N5. b This value N2…S3.
DFT Computational Results

The general approach was to do a full optimization at the DFT/6-31+G(2d,p) level with frequency checks, followed by DFT/6-311+G(2d,p). The latter repeatedly displayed imaginary frequencies that correspond to deformations towards the 'correct' geometries from the high-compliance methods. Re-optimization starting from the statically deformed geometries then led to fully converged DFT/6-311+G(2d,p) geometries without imaginary frequencies. A computed structure of 3 was first conducted with the B3LYP functional; although this optimized fully, the geometry indicated excessive repulsion between aryl substituents. Next, a series of functionals with differing approaches for inclusion of dispersion effects were tested, using primarily methods already validated for DTTA dimers in the work of Mou et al.: B3LYP-D3, B3LYP-D3BJ, M062X, O3LYP, and also the new APF-D method built into GW16.62. The most tractable method (good compromise between accuracy and efficiency) was B3LYP-D3BJ which was thenceforth used for all other calculations in conjunction with the above mentioned double and triple-ζ Pople basis sets. Cartesians coordinates of all the optimized geometries reported in this work are presented in Table S14.

Frontier Molecular Orbitals of the 'bicyclic' precursor 4.

Although it has a similar structure to the basal DTTA ring, the DFT calculations indicate that the FMOs of the cage compound are really quite different from those of the (monomeric or dimeric) DTTA rings. Notably, the LUMO of 4 is quite low-lying at -3.80 eV, compared to the HOMO at -7.65 eV. This LUMO is a π* fragment on the bridging "-N=S=N-" moiety. The HOMO by contrast is dominated by a p orbital framework mostly on the DTDA ring (at the two N atoms).
Frontier Molecular Orbitals of the triplet state of monomeric 3m

mCF3 triplet monomer

|                | E(ev) | gaps(eV) | E(AU) |
|----------------|-------|----------|-------|
| 83a L+1        | -1.30751 | 0.04805  |
| 82a L          | -2.03623 | 0.07483  |
| 81a H          | -6.02052 | 0.22125  |
| 80a H-1        | -6.5789  | 0.24177  |
| 79a H-2        | -7.9392  | 1.360298 |
| 78a H-3        | -8.00668 | 0.29424  |
| 77a H-4        | -8.7101  | 0.32009  |
| 76a H-5        | -9.04314 | 0.33233  |

Frontier Molecular Orbitals of the singlet C1 state of monomeric 3o

mCF3 singlet C1 monomer

|                | E(ev) | gaps(eV) | E(AU) |
|----------------|-------|----------|-------|
| 68a L+1        | -1.96929 | 0.07237  |
| 67a L          | -3.91926 | 1.4403   |
| 66a H          | -6.25155 | 2.22974  |
| 65a H-1        | -7.8192  | 1.567649 |
| 66a H-2        | -7.9577  | 0.138506 |
| 65a H-3        | -8.49703 | 0.31226  |
| 64a H-4        | -8.7833  | 0.32278  |
| 63a H-5        | -9.45079 | 0.34731  |
Frontier Molecular Orbitals of the dichloro precursor 5

Table S11  DFT Computed Results for the ‘parent’ HCN₃S₂ dimer

| Code | Geometry      | Rel E, kJ | Dimer E, kJ | dist i···i, Å | d(S-S)* | Torsion |
|------|---------------|-----------|-------------|---------------|---------|---------|
| 7a   | cofacial-0    | 0.0       | -119.0      | 2.788         | 2.5369  | 0.1     |
| 7c   | cofacial-64   | 6.1       | -112.9      | 2.683         | 2.0573  | 64.4    |
| 7d   | cofacial-149  | 5.5       | -113.5      | 2.772         | 2.6604  | 149.3   |
| 7d'  | cofacial-149  | 5.5       | -113.5      | 2.772         | 2.6586  | 149.3   |
| 7e   | S,S antarafacial | 65.9  | -53.1       | 3.234         | 2.4550  | 180.0   |
| 7f   | S,N antarafacial | 65.9  | -53.1       | 3.490         | 1.7985  | 155.3   |

Table S12  DFT Computed Results for the CF₃CN₃S₂ dimer

| Code | Geometry      | Rel E, kJ | Dimer E, kJ | dist ii···ii, Å | d(S-S)* | Torsion |
|------|---------------|-----------|-------------|-----------------|---------|---------|
| 8a   | cofacial-0    | 2.4       | -119.8      | 2.832           | 2.5248  | 0.1     |
| 8c   | cofacial-65   | 0.0       | -122.2      | 2.668           | 2.0803  | 64.8    |
| 8d   | cofacial-152  | 2.5       | -119.8      | 2.774           | 2.7279  | 152.4   |
| 8e   | S,S antarafacial | 72.4  | -54.7       | 3.206           | 2.456   | 180.0   |

Table S13  DFT Computed Results for the Me₂NCN₃S₂ dimer

| Code | Geometry      | Rel E, kJ | Dimer E, kJ | dist ii···ii, Å | d(S-S)* | Torsion |
|------|---------------|-----------|-------------|-----------------|---------|---------|
| 9a   | cofacial-4    | 0.2       | -0.8*       | 2.827           | 2.827   | 0       |
| 9c   | cofacial-64   | 0.4       | -0.6*       | 2.691           | 2.0612  | 65.1    |
| 9d   | cofacial-150  | 0.0       | -1.0        | 2.871           | 2.6893  | 149.6   |

* Never fully converges.
### Table S14  DFT Computed Cartesian Geometries with Structure Plots

#### 3a  DTTADIMER-B3LYPD3BJ-6311G2DP-OPT

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| S    | 3.428800 | -1.892200 | 0.084200 |
| S    | 3.515500 | 0.249100  | 1.863700 |
| F    | -2.474800 | -2.953800 | -1.448700 |
| F    | -3.590300 | -3.721800 | 0.245700 |
| N    | 1.842500  | -1.806200 | 0.363800 |
| N    | 1.920800  | 0.025500  | 1.916000 |
| N    | 4.320900  | -0.949600 | 1.108900 |
| F    | -4.255400 | -1.920200 | -0.756100 |
| C    | 1.294400  | -0.910800 | 1.194200 |
| C    | -0.174300 | -0.976600 | 1.355300 |
| C    | -2.318100 | -1.758300 | 0.593800 |
| C    | -2.952900 | -1.028300 | 1.596500 |
| H    | -4.031800 | -1.037100 | 1.673300 |
| C    | -0.938300 | -1.743200 | 0.473800 |
| H    | -0.446500 | -2.299400 | -0.309500 |
| C    | -2.192300 | -0.274600 | 2.478500 |
| H    | -2.680400 | 0.304900  | 3.250800 |
| C    | -0.810700 | -0.241300 | 2.356900 |
| H    | -0.214200 | 0.362300  | 3.026100 |
| C    | -3.150900 | -2.584400 | -0.342800 |
| S    | 3.515700  | -0.249300 | 1.863600 |
| S    | 3.429000  | 1.892000  | -0.084200 |
| F    | -2.474400 | 2.954000  | 1.448600 |
| N    | 1.842800  | 1.806200  | -0.363800 |
| N    | 1.921000  | -0.255000 | -1.916000 |
| N    | 4.321200  | 0.949300  | -1.100700 |
| C    | 1.294600  | 0.910900  | -1.194400 |
| C    | -0.174100 | 0.976700  | -1.355400 |
| C    | -0.810500 | 0.241300  | -2.356900 |
| H    | -0.214000 | -0.362200 | -3.026200 |
| C    | -0.938000 | 1.743300  | -0.473900 |
| H    | -0.446200 | 2.299500  | 0.309400 |
| C    | -2.317800 | 1.758500  | -0.593800 |
| C    | -2.192100 | 0.274600  | -2.478500 |
| H    | -2.680200 | -0.304800 | -3.250700 |
| C    | -2.952600 | 1.028400  | -1.596500 |
| H    | -4.031500 | 1.037200  | -1.673300 |
| C    | -3.150600 | 2.584600  | 0.342700 |

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#### 3a'  DTTADimer-B3LYPD3-6311

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| S    | 3.438300 | -1.900100 | 0.098800 |
| S    | 3.512500 | 0.249300  | 1.876100 |
DTTAdimer-m062x-6311G2dp-OF

S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
S       3.428700    1.828800    -0.250200
S       3.481800    -0.466100    -1.785700
F       -2.437400    2.929800    1.323000
F       -3.611200    3.587200    -0.357800
N       1.852300    1.760100    -0.533000
N       1.900600    -0.017200    -1.927000
N       4.325400    0.956000    -1.122500
H    -4.029200   0.925800   -1.680400  
C     -0.925100   1.670100   -0.539100  
H    -0.425200   2.254200     0.222400  
C    -2.196400   0.137200   -2.480900  
H    -2.693200   -0.467000   -3.231800  
C     -0.815000   0.107100   -2.369500  
H    -0.222200   -0.519900   -3.024700  
C     -3.129300   2.528700     0.272600  
S       3.482900   0.418600   -1.804200  
S       3.420400   -1.844500    0.221100  
F    -3.568700   -3.642700     0.345400  
F    -4.226900   -1.876800   -0.706900  
F    -2.448700   -2.925300   -1.358700  
N       1.843400   -1.767300    0.492100  
N       1.899700   0.188400   -1.886300  
N       4.296600   -0.834400    1.162000  
C     -0.172700   -0.874800    2.400400  
C    -0.815500   -0.107100    2.369500  
H    -0.222500    0.519800    3.024600  
C    -0.925800   -1.669800    0.538900  
H    -0.426000   -2.253800   -0.222800  
C    -2.305000   -1.676100    0.645800  
C    -2.196800   -0.137200    2.481000  
H    -2.692600    0.466900    3.232000  
C    -2.947800   -0.917400    1.616400  
H    -4.029700   -0.925700    1.680600  
C    -3.130000   -2.528300   -0.272700  
----------------------------------------

3a''' DTTAdimer_noDispersion_b3lyp6311G2dp_OF2

S       3.423400   1.828700    0.303600  
S       3.411800   0.107600   -1.884200  
F    -2.876400   2.952100    1.781200  
F    -2.428900   4.672000    0.543000  
N       1.837800   1.908000   -0.007300  
N       1.827300   0.423600   -1.883000  
N       4.270900   1.117700   -0.912500  
F    -4.272800   3.567700    0.237200  
C     -1.253600   1.249500   -1.000500  
C    -0.202000   1.487900   -1.180500  
C    -2.254000   2.536300   -0.465300  
C    -2.942100   1.937000   -1.515000  
H    -4.002000   2.112100   -1.639600  
C    -0.891600   2.317200   -0.296200  
H    -0.357000   2.785000    0.518900  
C    -2.254000   1.110600   -2.398500  
H    -2.785700   0.638200   -3.215200  
C    -0.896800   0.884800   -2.235400  

S21
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -0.3617 | 0.2412  | -2.9197 |
| C    | -2.9619 | 3.4294  | 0.5159  |
| S    | 3.3978  | -0.1839 | 1.8884  |
| S    | 3.3817  | -1.9052 | -0.2990 |
| F    | -3.8087 | -4.3032 | 0.1415  |
| F    | -3.9630 | -2.6405 | -1.2386 |
| F    | -2.2888 | -4.0143 | -1.3823 |
| N    | 1.7932  | -1.9484 | 0.0112  |
| N    | 1.8067  | -0.4634 | 1.8786  |
| N    | 4.2388  | -1.2137 | 0.9213  |
| C    | 1.2186  | -1.2767 | 0.9937  |
| C    | 0.2425  | -1.4827 | 1.1665  |
| C    | 0.9300  | -0.8563 | 2.2086  |
| H    | -0.3875 | -0.2158 | 2.8900  |
| C    | -0.9433 | -2.3094 | 0.2827  |
| H    | -0.4147 | -2.7964 | -0.5232 |
| C    | -2.3066 | -2.4995 | 0.4462  |
| C    | -2.2960 | -1.0538 | 2.3664  |
| H    | -2.8212 | -0.5620 | 3.1754  |
| C    | -2.9905 | -1.8744 | 1.4891  |
| H    | -4.0550 | -2.0302 | 1.6114  |
| C    | 3.0809  | -3.3662 | -0.5076 |

---

3a"""" O3LYP/6-311+G(3df)(2p) DTTADIMER-O3LYP-6311G2DP-OF1

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| S    | -3.3804 | -1.8240 | 0.4585  |
| S    | -3.4084 | -0.2989 | -1.8426 |
| F    | 2.4095  | -3.5391 | 1.8255  |
| F    | 3.2722  | -4.7147 | 0.2221  |
| N    | 1.8082  | -1.9610 | 0.1336  |
| N    | 1.8287  | -0.6214 | 1.8644  |
| N    | 4.2595  | -1.2367 | -0.8039 |
| F    | 4.2578  | -2.9045 | 0.8879  |
| C    | 1.2456  | -1.3939 | -0.9409 |
| C    | 0.1992  | -1.6784 | -1.1487 |
| C    | 2.2710  | -2.6545 | -0.3757 |
| C    | 2.9219  | -2.2052 | -1.5253 |
| H    | 3.9774  | -2.4049 | -1.6690 |
| C    | 0.9191  | -2.3995 | -0.1898 |
| H    | 0.4159  | -2.7483 | 0.7006  |
| C    | 2.2084  | -1.4938 | -2.4813 |
| H    | 2.7104  | -1.1392 | -3.3748 |
| C    | 0.8575  | -1.2281 | -2.2975 |
| H    | 0.3066  | -0.6685 | -3.0423 |
| C    | 3.0472  | -3.4495 | 0.6447  |
| S    | -3.4087 | -2.9810 | 1.8424  |
| S    | -3.3810 | 1.8233  | -0.4586 |
| F    | 3.2712  | 4.7153  | -0.2221 |
| F    | 4.2570  | 2.9052  | -0.8880 |
| F    | 2.4085  | 3.5396  | -1.8255 |
\[
\begin{array}{ccc}
S & -1.808900 & 1.960800 & -0.133600 \\
N & -1.829200 & 0.621200 & 1.864500 \\
N & -4.260000 & 1.235600 & 0.883600 \\
C & -1.246200 & 1.393900 & 0.941100 \\
C & 0.198600 & 1.678600 & 1.148800 \\
C & 0.856900 & 1.228400 & 2.297600 \\
H & 0.306100 & 0.668700 & 3.042400 \\
C & 0.918400 & 2.399800 & 0.189900 \\
H & 0.415000 & 2.748600 & -0.700400 \\
C & 2.270200 & 2.654900 & 0.375700 \\
C & 2.207900 & 1.494200 & 2.481400 \\
H & 2.709900 & 1.139700 & 3.374800 \\
C & 2.921300 & 2.205700 & 1.525300 \\
H & 3.976700 & 2.405500 & 1.669000 \\
C & 3.046300 & 3.450100 & -0.644600 \\
\end{array}
\]
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3b SYN COFACIAL - S-B3LYP3B3J - 6311G2DP - OF2

\[
\begin{array}{ccc}
S & -3.720200 & -1.126100 & 1.332400 \\
S & -2.923700 & -1.940900 & -1.209600 \\
F & 3.244500 & -2.356600 & -1.546200 \\
F & 4.772900 & -1.686100 & -0.154500 \\
N & -2.128800 & -1.024800 & 1.585000 \\
N & -1.445600 & -1.752000 & -0.603300 \\
N & -4.107800 & -1.867900 & -0.907000 \\
F & 3.781100 & -3.588600 & 0.154000 \\
C & -1.221600 & -1.328500 & 0.648900 \\
C & 0.198900 & -1.214200 & 1.045100 \\
C & 2.526300 & -1.637300 & 0.593400 \\
C & 2.886100 & -0.946800 & 1.746500 \\
H & 3.930000 & -0.836300 & 2.006100 \\
C & 1.192700 & -1.763900 & 0.235200 \\
H & 0.914800 & -2.280900 & -0.671400 \\
C & 1.895800 & -0.393200 & 2.548800 \\
H & 2.170800 & 0.156900 & 3.439200 \\
C & 0.559000 & -0.533200 & 2.289900 \\
H & -0.215800 & -0.101600 & 2.827200 \\
C & 3.580600 & -2.306100 & -0.242700 \\
S & -4.086800 & 1.228600 & 0.427000 \\
S & -3.083000 & 0.459400 & -2.055700 \\
F & 3.694100 & 2.783000 & -1.784200 \\
F & 4.413100 & 1.476900 & -0.211500 \\
F & 3.139600 & 0.686500 & -1.784700 \\
N & -1.693000 & 1.002700 & -1.441100 \\
N & -2.565700 & 1.691100 & 0.688700 \\
N & -4.394800 & 0.833900 & -1.124300 \\
C & -1.591600 & 1.523700 & -0.213100 \\
C & -0.250700 & 2.000600 & 0.191500 \\
\end{array}
\]
S
C       1.849200 -2.950000  1.019200
H       1.334200 -3.880900  1.220000
C       3.163000 -2.973100  0.559300
H       3.674300 -3.912100  0.400000
C       5.229400 -1.751100 -0.197900
----------------------------------------

3d SYN COFACIAL-150-B3LYPD3BJ-6311G2DP-OF
S  -0.076900 -1.605300  1.342500
S   0.606100  1.101100  1.538600
F  -6.038300 -2.157500 -0.228200
F  -7.562500 -0.862900  0.617800
N  -1.600800 -0.985400  1.140700
N  -0.929800  1.325500  1.085600
N   1.008200 -0.460900  1.712800
F  -7.031300 -0.682800 -1.474700
C  -1.827200  0.301700  1.006300
C  -3.221200  0.708500  0.716800
C  -5.474300  0.120900  0.111400
C  -5.841400  1.466800  0.137500
H  -6.860000  1.754400 -0.089200
C  -4.175700 -0.261300  0.398500
C  -3.886500 -1.300800  0.372200
C  -4.893600  2.428800  0.452400
H  -5.172800  3.474300  0.474500
C  -3.586400  2.054600  0.739300
H  -2.840100  2.797500  0.982900
C  -6.517300 -0.900700 -0.241500
S  -0.606100  1.101100 -1.538600
S   0.076900 -1.605300 -1.342400
F   7.562500 -0.862900 -0.617800
F   7.031300 -0.682800  1.474600
F  6.038300 -2.157500  0.228200
N   1.600800 -0.985400 -1.140700
N   0.929800  1.325500 -1.085600
N  -1.008300 -0.460900 -1.712800
C   1.827200  0.301700 -1.006300
C   3.221200  0.708500 -0.716800
C   3.586400  2.054600 -0.739300
H   2.840100  2.797500 -0.982900
C   4.175700 -0.261300 -0.398500
H   3.886500 -1.300800 -0.372200
C   5.474300  0.120900 -0.111400
C   4.893600  2.428800 -0.452400
H   5.172800  3.474300 -0.474500
C   5.841400  1.466800 -0.137500
H   6.860000  1.754400  0.089200
C   6.517300 -0.900700  0.241500
3d' Syn' Cofacial150- B3LYP3BJ-6311G2DP-OF
S 0.479800 -0.229900 -1.578400
S -0.178200 -2.938900 -1.336700
F -4.350600 3.244400 0.797000
F -5.175000 3.114900 -1.282000
N -1.014800 -0.013700 -1.003200
N -1.685400 -2.325000 -1.016400
N 0.870700 -1.790400 -1.789700
F -6.456100 2.789600 0.519900
C -1.903000 -1.039200 -0.860600
C -3.271300 -0.634300 -0.464400
C -4.891000 1.090400 -0.013400
C -5.838100 0.130200 0.320400
H -6.830000 0.432500 0.626200
C -3.611500 0.715100 -0.465600
H -2.872400 1.460000 -0.664100
C -5.496600 -1.218000 0.262300
H -6.229500 -1.969100 0.527000
C -4.223600 -1.601100 -0.125300
H -3.946200 -2.644800 -0.164200
C -5.223800 2.554600 0.028500
S 0.178200 -2.938900 1.336700
S -0.479800 -0.229900 1.578400
F 5.174900 3.114900 1.282000
F 6.456100 2.789600 0.519900
F 4.350700 3.244400 -0.797000
N 1.014800 -0.013700 1.003200
N 1.685400 -2.325000 1.016400
N -0.870700 -1.790400 1.789700
C 1.903000 -1.039200 0.860600
C 3.271300 -0.634300 0.464500
C 4.891000 -1.601100 0.125300
H 3.946200 -2.644800 0.164200
C 3.611500 0.715100 0.465600
H 2.872400 1.460000 0.664100
C 4.891000 1.090400 0.013400
C 5.496600 -1.218000 -0.262300
H 6.229500 -1.969100 -0.527000
C 5.838100 0.130200 -0.320400
H 6.830000 0.432500 -0.626200

3d'' AntiCofacial150-B3LYP3BJ-6311G2DP-OF
S -0.235000 0.478700 1.480500
S -0.301100 -2.303800 1.193500
F 5.423000 2.603200 -0.618200
|  | x     | y     | z     |
|---|-------|-------|-------|
| F | 6.1232 | 2.2132 | 1.3942 |
| N | 1.2864 | 0.3839 | 0.9644 |
| N | 1.3260 | -2.1024 | 0.9419 |
| N | -1.0301 | -0.9268 | 1.6369 |
| F | 7.3252 | 1.6025 | -0.3069 |
| C | 1.8791 | -0.9168 | 0.8260 |
| C | 3.3203 | -0.8803 | 0.4867 |
| C | 5.3527 | 0.3641 | 0.1372 |
| C | 6.0264 | -0.8056 | -0.1925 |
| H | 7.0739 | -0.7701 | -0.4574 |
| C | 4.0054 | 0.3323 | 0.4768 |
| C | 5.3403 | -2.0167 | 0.1580 |
| H | 5.8595 | -2.9296 | -0.4453 |
| C | 3.9972 | -2.0575 | 0.1520 |
| H | 3.4785 | 1.2408 | 0.7315 |
| C | 6.0602 | 1.6892 | 0.1483 |
| S | -0.5397 | -2.1696 | 1.4857 |
| S | 0.8207 | 0.2708 | 1.6426 |
| F | -6.3801 | -1.2019 | 0.3266 |
| F | -6.9568 | 0.4622 | 1.5968 |
| F | -7.5272 | 0.4494 | 0.4931 |
| N | -0.5859 | 0.8702 | -1.1777 |
| N | -1.8406 | -1.1820 | -1.2827 |
| N | 0.7931 | -1.3348 | -1.8752 |
| C | -1.7174 | 0.1139 | -1.0263 |
| C | -2.9446 | 0.8601 | -0.6672 |
| C | -2.9402 | 2.2546 | -0.6265 |
| H | -2.0311 | 2.7847 | -0.8728 |
| C | -4.1124 | 0.1630 | -0.3460 |
| H | -4.1087 | -0.9160 | -0.3686 |
| C | -5.2542 | 0.8608 | 0.0067 |
| C | -4.0922 | 2.9467 | 0.2733 |
| H | -4.0843 | 4.0287 | -0.2453 |
| C | -5.2516 | 2.2556 | 0.0444 |
| H | -6.1500 | 2.7910 | 0.3233 |
| C | -6.5217 | 0.1355 | 0.3576 |

3e  ANTARAFACIAL2-B3LYP3DJ-6-311G2DP-OF

|  | x     | y     | z     |
|---|-------|-------|-------|
| S | 0.1519 | -1.5900 | -0.9417 |
| S | 0.7800 | 1.0859 | -1.2837 |
| F | 6.7256 | 2.1036 | -0.1760 |
| F | 7.8844 | 0.9708 | 1.2695 |
| N | 1.7140 | -1.7225 | -0.5329 |
| N | 2.2613 | 0.6136 | -0.8304 |
| N | -0.1613 | -0.1858 | -1.7466 |
| F | 8.2148 | 0.6753 | -0.8510 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 2.535100| -0.66100| -0.544600|
| C    | 3.955800| -0.958200| -0.235700|
| C    | 6.221100| -0.281200| 0.067200|
| C    | 6.626800| -1.582700| 0.359900|
| H    | 7.664200| -1.707400| 0.591400|
| C    | 4.897100| 0.075000| -0.229100|
| H    | 4.581800| 1.082100| -0.454900|
| C    | 5.692500| -2.528200| 0.354600|
| H    | 6.001400| -3.540200| 0.582600|
| C    | 4.362700| 2.260800| -0.058400|
| H    | 3.628800| 3.054000| -0.053300|
| C    | 4.897100| -0.075000| 0.229200|
| H    | 4.581800| -1.082100| 0.454700|
| C    | 6.221100| 0.201000| -0.067100|
| C    | 6.626800| -0.067100| -0.354000|
| H    | 7.964900| 1.397700| -0.322100|

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3f  SN-antarafacial-B3LYPD3BJ-6311-G2DP-OF

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| S    | 0.661300| -0.944100| -0.521500|
| S    | 0.300700| 1.695900| -0.578300|
| F    | 6.648300| -2.377400| -0.265900|
| F    | 8.139900| -1.200700| -1.317900|
| N    | 2.241800| -0.579700| -0.489500|
| N    | 1.917000| 1.802200| -0.412900|
| N    | -0.163800| 0.270500| -1.250300|
| F    | 8.065300| -1.165400| 0.847000|
| C    | 2.658200| 0.691000| -0.401100|
| C    | 4.127500| 0.890700| -0.380400|
| C    | 6.352300| -0.025100| -0.314800|
| C    | 6.891300| 1.260700| -0.338000|
| H    | 7.964900| 1.397700| -0.322100|
3m Monomer-6-31G-triplet

| Atom | X  | Y  | Z   |
|------|----|----|-----|
| S    | -3.047700 | -1.800800 | -0.018900 |
| S    | -3.963200 | 0.871500  | -0.009000 |
| F    | 3.090200  | -1.989000 | 0.027400  |
| F    | 4.274700  | -0.551500 | -1.087800 |
| N    | -1.597400 | -1.074300 | -0.058900 |
| N    | -2.371700 | 1.188500  | -0.050200 |
| N    | -4.306700 | -0.739500 | 0.157200  |
| F    | 4.299000  | -0.522800 | 1.078100  |
| C    | -1.418800 | 0.250500  | -0.034900 |
| C    | -0.018800 | 0.729200  | -0.017500 |
| C    | 2.344400  | 0.263100  | 0.066400  |
| C    | 2.625300  | 1.628700  | 0.021800  |
| H    | 3.651900  | 1.971100  | 0.037800  |
| C    | 1.035600  | -0.189100 | -0.013100 |
| H    | 0.820800  | -1.246900 | -0.025100 |
| C    | 1.579300  | 2.540200  | 0.018800  |
| H    | 1.789700  | 3.601900  | 0.030100  |
| C    | 0.263600  | 2.096800  | -0.001600 |
4a  MCF3BICYCLIC-B3LYP3B1_6311GPLUS2DP-OF

5a  mCF3dichloride_6311D3bj_OF
|    | C       | Cl      | Cl      |
|----|---------|---------|---------|
|    | 4.293200 | -3.895500 | -2.836000 |
|    | -0.707700 | 1.178700 | -2.228000 |
|    | 0.096600  | 1.244900 | 1.068400 |

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**7a**  
H-TTADIMER-B3LYPD3BJ-6311G2DP-OF

|    | S       | Cl      | Cl      |
|----|---------|---------|---------|
|    | -1.269900 | -3.895500 | -2.836000 |
|    | 1.397000  | 1.178700 | -2.228000 |
|    | -0.543700 | 1.058200 | 1.068400 |

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**7c**  
COFACIAL-60-B3LYPD3BJ-6311G2DP-OF

|    | S       | Cl      | Cl      |
|----|---------|---------|---------|
|    | -0.856900 | -1.686100 | -1.459400 |
|    | 0.975800  | 1.168600 | 0.000400 |
|    | -1.288700 | 1.056000 | 1.610100 |

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**7d**  
H-COFACIAL150-B3LYPD3BJ-6311G2DP-OF

|    | S       | Cl      | Cl      |
|----|---------|---------|---------|
|    | -1.324000 | -1.439200 | -1.228600 |
|    | 1.500700  | -1.213300 | -0.789100 |
|    | -0.128300 | -0.835000 | 2.672500 |
|    | 0.096600  | 1.244900 | 1.068400 |
S       1.324000 1.500700 0.128300
N       1.346500 0.880700 -1.424600
N       1.225700 -1.443500 -0.755600
N       1.559500 -0.355500 1.248800
C       1.267700 -0.406500 -1.628200
H       1.228600 -0.709100 -2.672500
----------------------------------------
7d'  H-COFACIAL150SYMPRIME-B3LYPD3B3J-6311G2DP-OF
S       1.439700 -1.213100 -0.835200
S       1.323300 1.500600 -0.127100
N       1.225500 -1.443700 0.755200
N       1.345700 0.880000 1.425200
N       1.560000 -0.755600 1.248800
C       1.266900 -0.407400 1.628300
S       1.439900 -1.212900 0.835200
S       1.323100 1.500800 0.127000
N       1.226000 -1.443600 -0.755200
N       1.345400 0.880100 -1.425200
N       1.559900 -0.755200 1.248500
C       1.267100 -0.407200 1.628300
H       1.227500 -0.710400 -2.672500
H       1.227700 -0.710300 -2.672500
----------------------------------------
7e  H-ANTARAFACIAL-B3LYPD3B3J-6311G2DP-O
S       -1.005900 -1.387000 0.783700
S       -1.005600 1.387000 0.703800
N       -2.129200 -1.216400 -0.471200
N       -2.128700 1.216800 -0.471200
N       -0.829200 0.000000 1.578600
C       -2.526800 0.000200 -0.831700
H       -3.355800 0.000400 -1.536700
S       1.005900 1.387000 -0.703700
S       1.005500 -1.387000 -0.703800
N       2.128700 -1.216800 0.471200
N       2.129200 1.216400 0.471200
N       0.829200 0.000000 1.578600
C       2.526800 -0.000300 0.831700
H       3.355800 0.000400 1.536700
----------------------------------------
7f  SN-antarafacial-B3LYPD3B3J-6311-G2DP-OF
S       -0.702000 -1.263000 0.613700
S       -1.458500 1.299600 0.533000
N       -2.032000 -1.532800 -0.310700
N       -2.700300 0.787400 -0.483300
N       -0.886000 0.099300 1.505000
----------------------------------------
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -2.821600  | -0.515200  | -0.629500  |
| S    | 0.497300   | 0.964800   | -1.051100  |
| S    | 2.128400   | -1.270100  | -0.371600  |
| N    | 2.772400   | -0.215600  | 0.775100   |
| N    | 1.713000   | 1.634000   | -0.389300  |
| N    | 0.463000   | -0.743100  | -0.654000  |
| C    | 2.487000   | 1.042400   | 0.637000   |
| H    | -3.726300  | -0.798400  | -1.164800  |
| H    | 2.979700   | 1.732400   | 1.317400   |

7 HCN3S2 MON-B3LYPD36311G2DP-TRIPLET-ENVELOPE-OP

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| S    | -1.419400  | -0.552300  | -0.038000  |
| S    | 1.419400   | -0.552200  | -0.038000  |
| N    | -1.204000  | 1.069700   | -0.005600  |
| N    | 1.204000   | 1.069700   | -0.005600  |
| N    | 0.000000   | -1.398700  | 0.132600   |
| C    | 0.000000   | 1.628800   | 0.043400   |
| H    | 0.001000   | 2.714400   | 0.105400   |

7 HCN3S2 monomer-b3lypD3BJ6311G2dp-singletC1-OP

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| S    | -1.362500  | -0.531600  | -0.073100  |
| S    | 1.403900   | -0.558100  | 0.166800   |
| N    | -1.175500  | 0.970400   | 0.390700   |
| N    | 1.150200   | 1.120000   | -0.279100  |
| N    | 0.041600   | -1.352900  | -0.214200  |
| C    | 0.163800   | 1.474400   | 1.215200   |

8a CF3 Cofacial-0 DIMER-B3LYPD3BJ-6311G2DP-OF

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| S    | 1.762700   | -1.265000  | -1.395100  |
| S    | 1.742200   | -1.259400  | 1.399200   |
| N    | 0.163800   | -1.474400  | -1.215200  |
| N    | 0.149000   | -1.460100  | 1.195200   |
| N    | 2.590500   | -1.451300  | 0.089100   |
| C    | -0.384500  | -1.556800  | -0.014800  |
| S    | 1.741800   | 1.259800   | -1.399200  |
| S    | 1.762400   | 1.265400   | 1.395100   |
| N    | 0.163300   | 1.474400   | 1.215200   |
| N    | 0.148600   | 1.460000   | -1.195200  |
| N    | 2.590100   | 1.451900   | -0.089100  |
| C    | -0.385000  | 1.556500   | 0.014800   |
| C    | -1.873000  | 1.933100   | 0.003400   |
| C    | -1.872500  | -1.933600  | -0.003400  |
| F    | -1.996200  | 3.246800   | -0.279600  |
| F    | -2.450100  | 1.711400   | 1.183400   |
8c CF3-COFA\text{\textsc{CIAL-65-B3LYP3BJ-6311-G2DP-OF}}

\begin{align*}
S & -2.537500 & 1.250000 & -0.934500 \\
F & -2.449700 & -1.711600 & -1.183300 \\
F & -1.995600 & -3.247300 & 0.279300 \\
F & -2.537000 & -1.250600 & 0.934700 \\
\end{align*}

\begin{align*}
S & 0.899100 & -2.429200 & -0.267900 \\
F & -0.237600 & -0.597000 & -2.049600 \\
N & 1.816800 & -1.163500 & 0.168700 \\
N & 0.770300 & 0.429800 & -1.30100 \\
N & 0.036100 & -2.153100 & -1.626000 \\
C & 1.618900 & 0.034700 & -0.376100 \\
S & -0.243400 & -0.863600 & 2.148000 \\
S & -2.034300 & -1.926500 & 0.237500 \\
N & -2.000500 & -0.863600 & -0.346000 \\
N & -0.731900 & 0.529500 & 1.467700 \\
N & -0.600500 & -2.161100 & 1.148800 \\
C & -1.459900 & 0.604800 & 0.388400 \\
C & -1.825800 & 2.013600 & 0.079800 \\
C & 2.580000 & 1.109300 & 0.138500 \\
F & 3.815500 & 0.892500 & -0.368700 \\
F & 2.681900 & 1.064300 & 1.474300 \\
F & 2.199700 & 2.332500 & -0.217100 \\
F & -0.954600 & 2.925300 & 0.350300 \\
F & -3.044800 & 2.349600 & 0.392300 \\
F & -1.885400 & 2.081800 & -1.420500 \\
\end{align*}

----------------------------------------

8d CF3-COFA\text{\textsc{CIAL-152-B3LYP3BJ-6311G2DP-OF}}

\begin{align*}
S & 0.381500 & -1.309500 & 1.795900 \\
S & -0.140000 & -1.624700 & -0.949000 \\
N & 1.822600 & -0.678300 & 1.222800 \\
N & 1.220200 & -0.756500 & -1.115900 \\
N & -0.506000 & -1.937000 & 0.593200 \\
C & 2.013700 & -0.498400 & -0.045600 \\
S & 0.140100 & 1.624600 & -0.949000 \\
S & -0.381500 & 1.309500 & 1.795900 \\
N & -1.822600 & 0.678300 & 1.222800 \\
N & -1.220200 & 0.756500 & -1.115900 \\
N & 0.506000 & 1.937000 & 0.593200 \\
C & -2.013700 & 0.498400 & -0.045600 \\
C & 3.385500 & 0.067400 & -0.438500 \\
C & -3.385500 & -0.067400 & -0.438500 \\
F & -3.259700 & -1.050400 & -0.949000 \\
F & -4.045100 & -0.552200 & 0.611800 \\
F & 4.045100 & 0.552200 & 0.611800 \\
F & 4.132600 & -0.905000 & -0.993100 \\
\end{align*}

S35
8e  CF3 S,Santarafacial-OF
S  -0.638200 -1.390600  1.048500
S  -0.638500  1.389400  1.049700
N  -2.126800 -1.212500  0.405700
N  -2.126800  1.212500  0.405700
N  -0.121900  0.000000  1.764300
C  -2.625100 -0.000500  0.223600
C  -4.104700  0.000000 -0.199500
F  -4.403200  1.081000 -0.925200
F  -4.406200 -1.084400 -0.918600
F  -4.885400  0.004400  0.897900
S  0.638200  1.390700 -1.048500
S  0.638500 -1.389400 -1.049700
N  2.126800 -1.212500 -0.405800
N  2.126800  1.213500 -0.405700
N  0.121900  0.000800  1.764300
C  2.625100  0.000500 -0.223600
C  4.104700  0.000000  0.199500
F  4.885400 -0.004500 -0.897900
F  4.403200 -1.089900  0.925300
F  4.406300  1.084500  0.918500

8o  CF3MONOMER-B3LYPD36311G2DP-SINGLET-OF
S  -1.922500  1.353600 -0.120700
S  -1.615600 -1.410100  0.082000
F  2.438800  1.234200  0.252000
F  2.156500 -0.750400  1.083000
N  -0.187900  1.248500  0.079000
N  -0.193700  1.248500 -0.079000
N  0.015200  1.472000 -1.207200
N  0.014700  1.475000  1.262000
N  -2.419000  1.510000 -0.000900
C  0.607200  1.590200 -0.000400
C  1.883100  0.043700  0.032200

9a  ME2NDIMER-Cofacial0-6311G2DP-OF-QC
S  -1.570600  1.256800 -1.387800
S  -1.571100  1.258300  1.386400
N  0.015200  1.472000 -1.207200
N  0.014700  1.475000  1.262000
N  -2.419000  1.510000 -0.000900
C  0.607200  1.590200 -0.000400
S  -1.573000 -1.256800 -1.386300
9o  ME2NMONOMER-B3LYPD3631G2DP-SINGLET-OF
S  1.563700  -1.343600  -0.231800
S  1.562700   1.343800   0.231800
N  0.024700  -1.153100   0.314100
N  0.024900   1.152700  -0.315400
N  2.432500   0.000600   0.001100
C  -0.605400   0.000500  -0.000700
N  -1.951800  -0.000200  -0.000300
C  -2.717700  -1.219200   0.199800
H  -2.054400  -2.075700   0.136000
H  -3.197900  -1.212400   1.182300
H  -3.493500  -1.287100  -0.566600
C  -2.717600   1.219100  -0.199100
H  -3.491000   1.288200   0.569600
H  -2.053700   2.075300  -0.138100
H  -3.200800   1.211500  -1.180100