Electronic Supplementary Information

Why do A•T and G•C Self-Sort? Hückel Aromaticity as a Driving Force for Electronic Complementarity in Base Pairing

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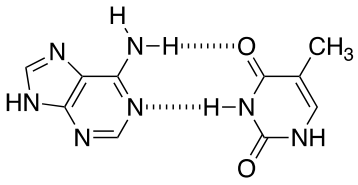
Details of computational methods.

DFT calculations. All geometries were optimized with a constrained C_s symmetry at ωB97X-D/6-311+G(d,p) level using ultrafine grid employing the Gaussian09 program. Vibrational frequency calculations verified the nature of the stationary points, and the reported gas-phase interaction energies for all 57 base pairs (see Figure S1) and the reference dimers (see Figures 3 and 4 in the main text), 1•1, 2•2, 3•3, 4•4, 5•5, 3•1, 6•4, include zero-point vibrational energy (ZPE) corrections. Planarization energies for bases, base pairs, and acyclic references with nonplanar C_1 minima structures (bases and base pairs with imaginary frequencies of at least 50*i* cm^{-1} at C_s symmetry: C, G, 8-oxoG, yC, IsoG, IsoC, K, Pi, G*, 6-thioG, 2-aminoA, 1, 2, 5, 6, G•U, 8-oxoG•A, reverse G•U, K•Pi, reverse G•C, $G•A_{imino}$, syn-G•A, G•A, G•4-thioU, G•2-thioU, G•G 3, G•6-thioG 3, 6-thioG•G 3, G•A 2, G•A 4, 8-oxoG•G, 1•1, 2•2, 5•5, 3•1, 6•4) were computed at the same ωB97X-D/6-311+G(d,p) level and listed in Table S3. The computed planarization energies for all nonplanar minima were less than 3 kcal/mol, except for the following: 1 (4.67 kcal/mol), 5 (3.22 kcal/mol), 6 (3.47 kcal/mol), reversed G•C (4.70 kcal/mol), 1•1 (3.47 kcal/mol), 5•5 (4.89 kcal/mol), and 6•4 (3.41 kcal/mol). Electrostatic potential (ESP) derived charges were computed for the planar geometries of A•T, G•C, A•A, I•I, and their isolated bases at ωB97X-D/6-311+G(d,p), using the pop=chelpg keyword in Gaussian09.

Block-localized wavefunction (BLW). BLW computations quantified the π-electron delocalization energies (DE_π) of all isolated bases and hydrogen-bonded bases and were performed at the B3LYP/6-31G(d) level using the GAMESS-2013-R1 program. The DE_π values were computed by the energy difference between the fully delocalized wavefunction (ψ_{deloc}) and the energy of a π-electron-localized wavefunction (ψ_{loc}) of the system considered; $DE_\pi = E(\psi_{loc}) - E(\psi_{deloc})$. Ψ_{loc} was computed by assigning all of the π-bonds and π-type lone-pairs to separate subspaces ("blocks") to disable π-electron delocalization. Based on this localization scheme, ψ_{loc} was computed by restricting the expansion of molecular orbitals over basis functions within a selected molecular subspace. Each block included two π-electrons and the p_z, d_{xz}, d_{yz} basis functions belonging to the heavy atoms assigned to the specific subspace. Direct comparisons of the computed DE_π values for the base pairs to the interacting bases provided a measure of the π-conjugation gain in the paired bases; $\Delta DE_\pi = DE_{a•b} - (DE_a + DE_b)$. The computed ΔDE_π values for all 57 base pairs were positive, indicating increased π-conjugation for all paired bases upon hydrogen bonding. However, the degree of π-conjugation gain differs depending on the degree of gain or loss in aromatic character in the paired bases. Higher ΔDE_π values indicate more aromaticity gain upon base pairing, lower ΔDE_π values indicate little to no change in aromatic character.

Natural Bond Orbital (NBO) analysis. NBO computations were performed at ωB97X-D/Def2-TZVPP//ωB97X-D/6-311+G(d,p) in the gas-phase using the planar geometries of selected isolated bases and hydrogen-bonded bases, to provide complementary insight. According to the NBO deletion procedure, all π* orbitals were deleted to quantify the effects of π-electron delocalization (DEL_π) for each of the selected hydrogen-bonded base (A•B) and the isolated bases (A and B). The difference, ΔNBO-DEL_π, calculated by the computed DEL_π of the complex minus that of its isolated nucleobases, provided a measure of the degree of increased π-electron delocalization in the monomers upon hydrogen bonding; $\Delta\text{NBO-}DEL_\pi = DEL_{\pi(A•B)} - [DEL_{\pi(A)} + DEL_{\pi(B)}]$.

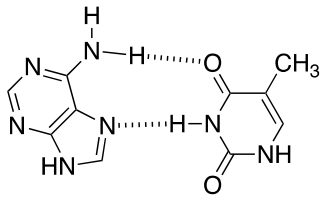
Doubly hydrogen-bonded pairs:



A•T

$-\Delta E$ = 15.06 kcal/mol

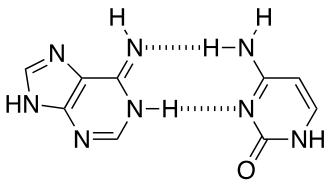
ΔDE_{π} = 10.15 kcal/mol



A•T(Hoog)

$-\Delta E$ = 15.58 kcal/mol

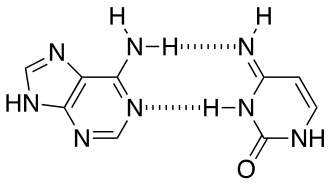
ΔDE_{π} = 12.18 kcal/mol



A_{imino}•C

$-\Delta E$ = 22.79 kcal/mol

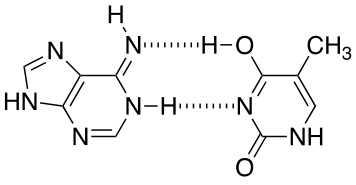
ΔDE_{π} = 20.12 kcal/mol



A•C_{imino}

$-\Delta E$ = 15.79 kcal/mol

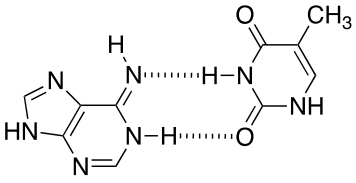
ΔDE_{π} = 10.09 kcal/mol



A_{imino}•T_{enol}

$-\Delta E$ = 28.05 kcal/mol

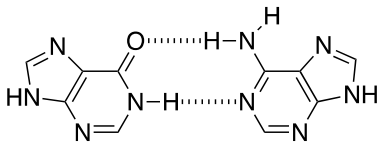
ΔDE_{π} = 25.19 kcal/mol



A_{imino}•T

$-\Delta E$ = 17.66 kcal/mol

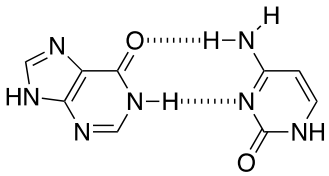
ΔDE_{π} = 13.61 kcal/mol



I•A

$-\Delta E$ = 16.25 kcal/mol

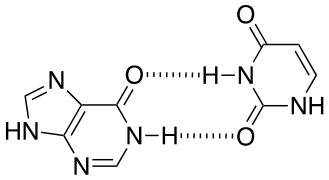
ΔDE_{π} = 13.47 kcal/mol



I•C

$-\Delta E$ = 21.96 kcal/mol

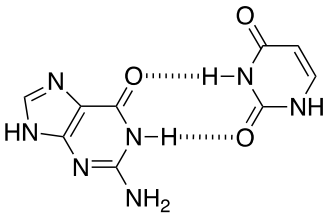
ΔDE_{π} = 19.89 kcal/mol



I•U

$-\Delta E$ = 14.60 kcal/mol

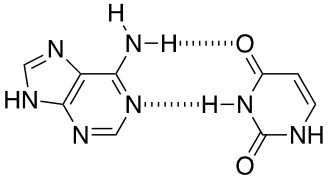
ΔDE_{π} = 12.92 kcal/mol



G•U

$-\Delta E$ = 16.32 kcal/mol

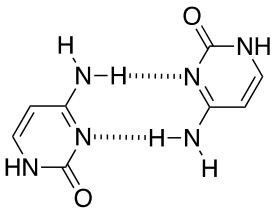
ΔDE_{π} = 14.36 kcal/mol



A•U

$-\Delta E$ = 15.14 kcal/mol

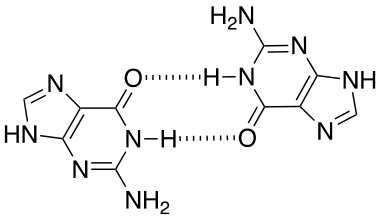
ΔDE_{π} = 10.26 kcal/mol



C•C

$-\Delta E$ = 20.18 kcal/mol

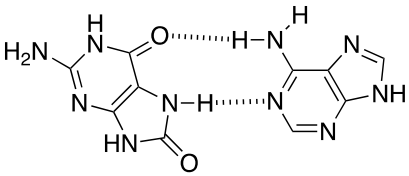
ΔDE_{π} = 19.48 kcal/mol



G•G

$-\Delta E$ = 27.10 kcal/mol

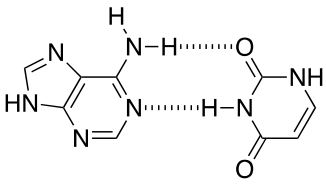
ΔDE_{π} = 28.33 kcal/mol



8-oxoG•A

$-\Delta E$ = 15.58 kcal/mol

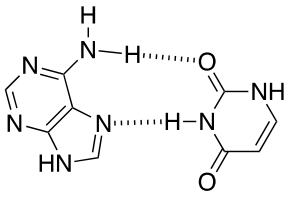
ΔDE_{π} = 12.28 kcal/mol



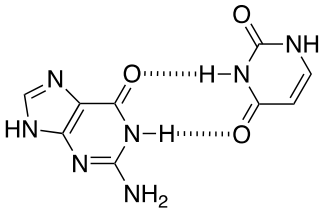
Reverse A•U

$-\Delta E$ = 14.67 kcal/mol

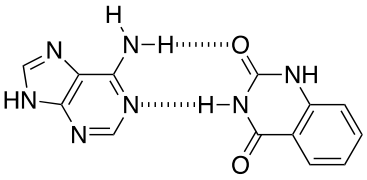
ΔDE_{π} = 9.19 kcal/mol



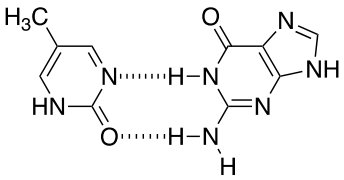
Reverse A•U(Hoog)
$-\Delta E$ = 15.31 kcal/mol
ΔDE_{π} = 11.52 kcal/mol



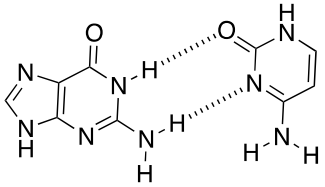
Reverse G•U
$-\Delta E$ = 17.43 kcal/mol
ΔDE_{π} = 17.12 kcal/mol



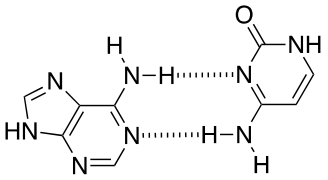
A•yT
$-\Delta E$ = 14.96 kcal/mol
ΔDE_{π} = 9.44 kcal/mol



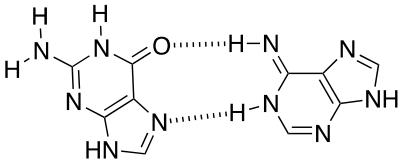
T(h)•G
$-\Delta E$ = 19.64 kcal/mol
ΔDE_{π} = 13.58 kcal/mol



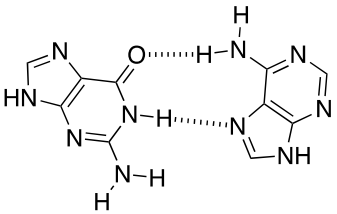
Reverse G•C
$-\Delta E$ = 14.11 kcal/mol
ΔDE_{π} = 10.13 kcal/mol



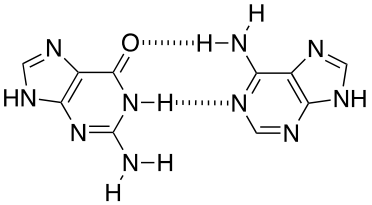
Reverse A•C
$-\Delta E$ = 15.62 kcal/mol
ΔDE_{π} = 13.06 kcal/mol



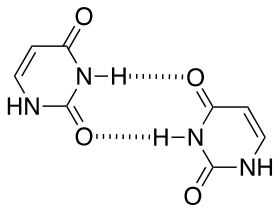
G•A_{imino}
$-\Delta E$ = 6.62 kcal/mol
ΔDE_{π} = 5.11 kcal/mol



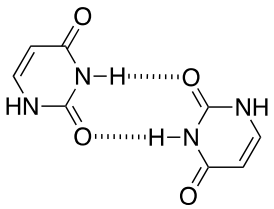
Syn-G•A
$-\Delta E$ = 14.65 kcal/mol
ΔDE_{π} = 14.59 kcal/mol



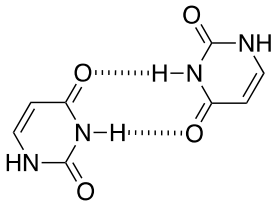
G•A
$-\Delta E$ = 16.73 kcal/mol
ΔDE_{π} = 13.95 kcal/mol



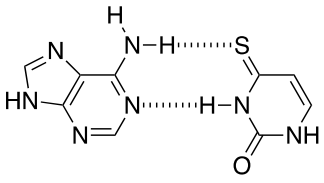
U•U 1
$-\Delta E$ = 12.18 kcal/mol
ΔDE_{π} = 10.22 kcal/mol



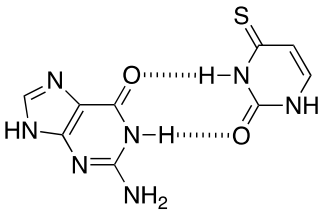
U•U 2
$-\Delta E$ = 11.73 kcal/mol
ΔDE_{π} = 9.25 kcal/mol



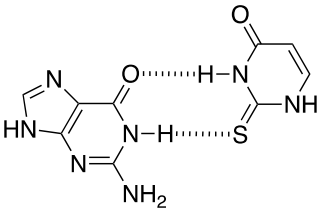
U•U 3
$-\Delta E$ = 12.68 kcal/mol
ΔDE_{π} = 11.41 kcal/mol



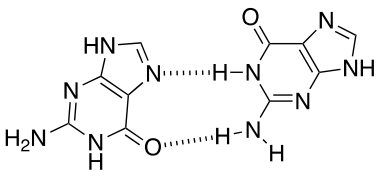
A•4-thioU
$-\Delta E$ = 13.92 kcal/mol
ΔDE_{π} = 8.69 kcal/mol



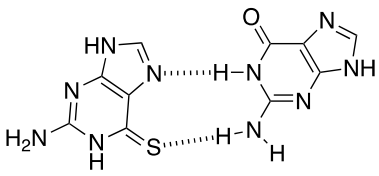
G•4-thioU
$-\Delta E$ = 15.69 kcal/mol
ΔDE_{π} = 13.14 kcal/mol



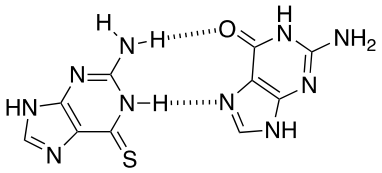
G•2-thioU
$-\Delta E$ = 14.14 kcal/mol
ΔDE_{π} = 15.04 kcal/mol



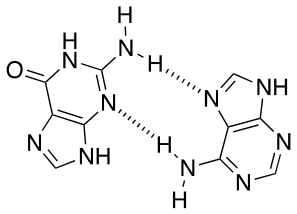
G•G 3
$-\Delta E$ = 20.08 kcal/mol
ΔDE_{π} = 14.20 kcal/mol



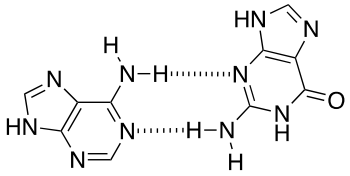
G•6-thioG 3
$-\Delta E$ = 20.49 kcal/mol
ΔDE_{π} = 15.01 kcal/mol



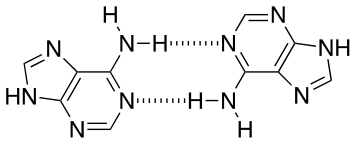
6-thioG•G 3
$-\Delta E$ = 20.97 kcal/mol
ΔDE_{π} = 16.63 kcal/mol



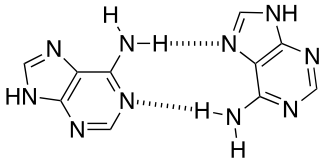
G•A 2
$-\Delta E$ = 11.46 kcal/mol
ΔDE_{π} = 8.63 kcal/mol



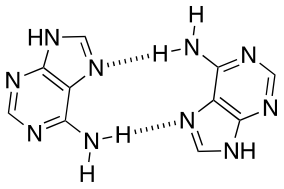
G•A 4
$-\Delta E$ = 12.84 kcal/mol
ΔDE_{π} = 8.34 kcal/mol



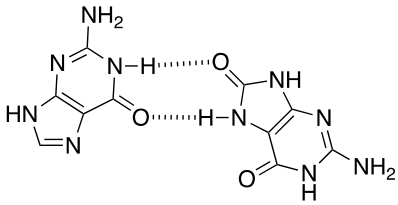
A•A 1
$-\Delta E$ = 12.76 kcal/mol
ΔDE_{π} = 8.60 kcal/mol



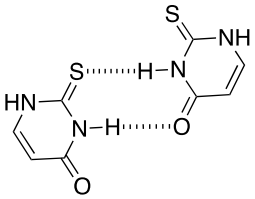
A•A 2
$-\Delta E$ = 11.82 kcal/mol
ΔDE_{π} = 9.20 kcal/mol



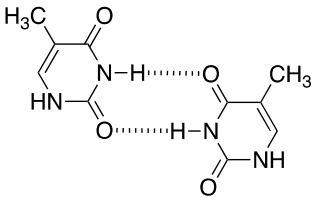
A•A 3
$-\Delta E$ = 10.26 kcal/mol
ΔDE_{π} = 9.16 kcal/mol



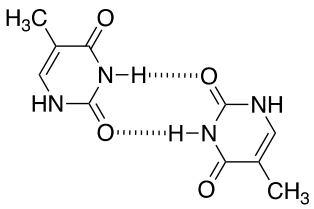
8-oxoG•G
$-\Delta E$ = 19.01 kcal/mol
ΔDE_{π} = 17.59 kcal/mol



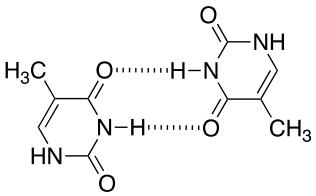
2-thioU•2-thioU
$-\Delta E$ = 10.61 kcal/mol
ΔDE_{π} = 9.53 kcal/mol



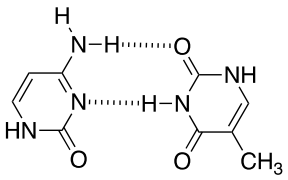
T•T 1
$-\Delta E$ = 12.37 kcal/mol
ΔDE_{π} = 10.47 kcal/mol



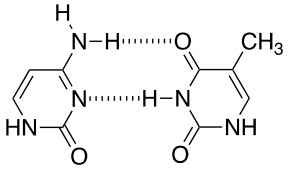
T•T 2
$-\Delta E$ = 12.07 kcal/mol
ΔDE_{π} = 9.65 kcal/mol



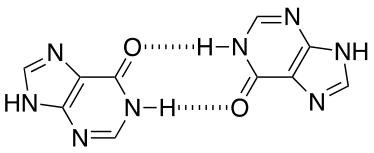
T•T 3
$-\Delta E$ = 12.69 kcal/mol
ΔDE_{π} = 11.36 kcal/mol



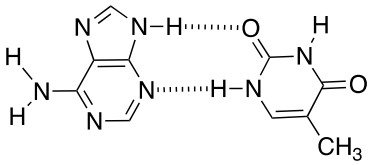
T•C 1
$-\Delta E$ = 12.03 kcal/mol
ΔDE_{π} = 9.41 kcal/mol



T•C 2
$-\Delta E$ = 12.64 kcal/mol
ΔDE_{π} = 10.97 kcal/mol

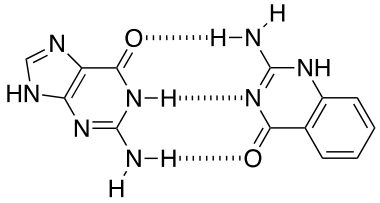


I•I
$-\Delta E$ = 20.63 kcal/mol
ΔDE_{π} = 20.06 kcal/mol

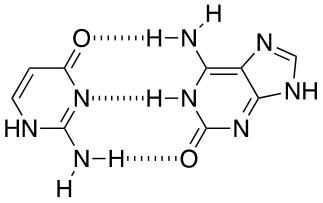


A•T(Hoog')
$-\Delta E$ = 18.62 kcal/mol
ΔDE_{π} = 16.73 kcal/mol

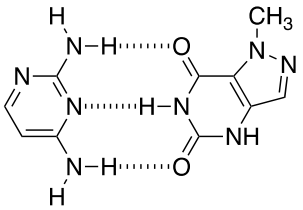
Triply hydrogen-bonded pairs:



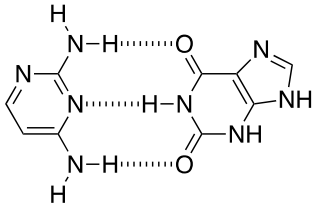
G•yC
$-\Delta E$ = 30.36 kcal/mol
ΔDE_{π} = 31.12 kcal/mol



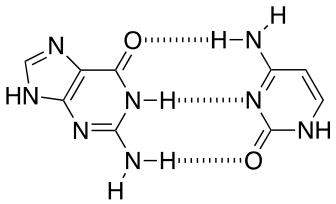
IsoC•IsoG
$-\Delta E$ = 32.87 kcal/mol
ΔDE_{π} = 42.85 kcal/mol



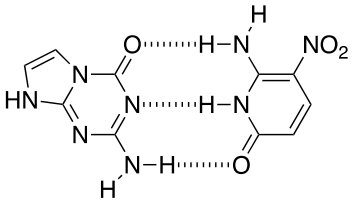
K•Pi
$-\Delta E$ = 16.99 kcal/mol
ΔDE_{π} = 13.84 kcal/mol



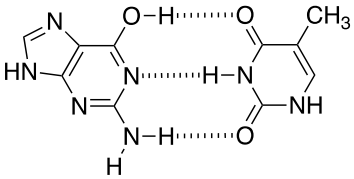
K•X
$-\Delta E$ = 16.76 kcal/mol
ΔDE_{π} = 13.47 kcal/mol



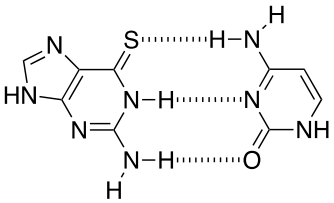
G•C
$-\Delta E$ = 28.05 kcal/mol
ΔDE_{π} = 28.37 kcal/mol



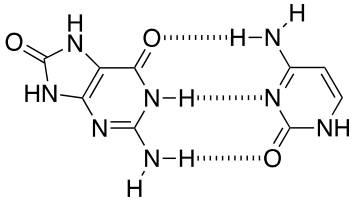
P•Z
$-\Delta E$ = 28.27 kcal/mol
ΔDE_{π} = 30.75 kcal/mol



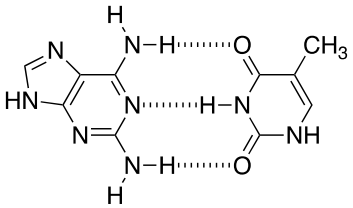
G*•T
$-\Delta E$ = 18.99 kcal/mol
ΔDE_{π} = 14.42 kcal/mol



6-thioG•C
$-\Delta E$ = 25.88 kcal/mol
ΔDE_{π} = 28.68 kcal/mol



8-oxoG•C
$-\Delta E$ = 28.75 kcal/mol
ΔDE_{π} = 30.70 kcal/mol



2-aminoA•T
$-\Delta E$ = 17.51 kcal/mol
ΔDE_{π} = 13.75 kcal/mol

Figure S1. Structures for all nucleobase pairs considered.

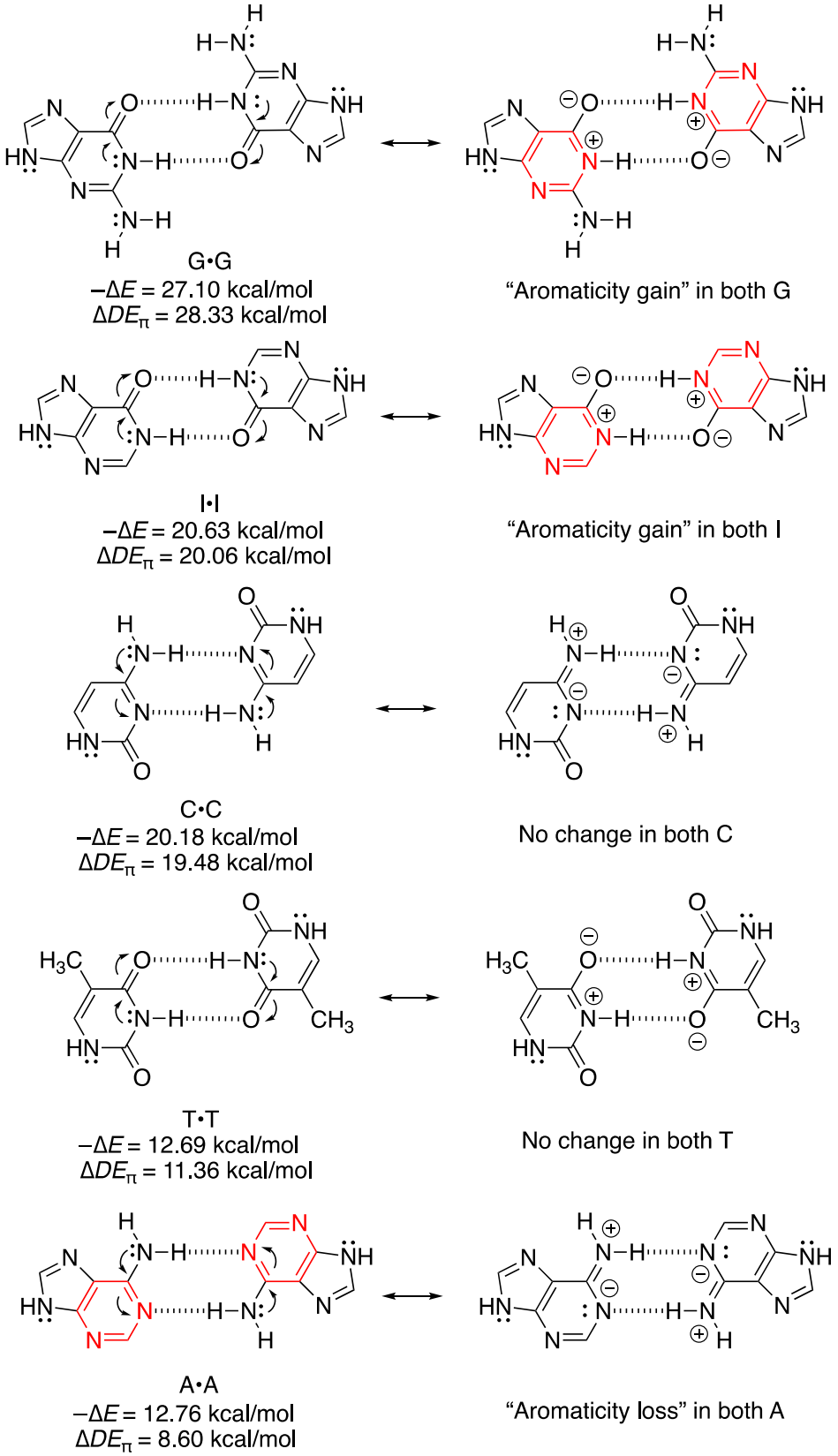


Figure S2. Resonance forms for base pairs shown in Figure 4 of the main text.

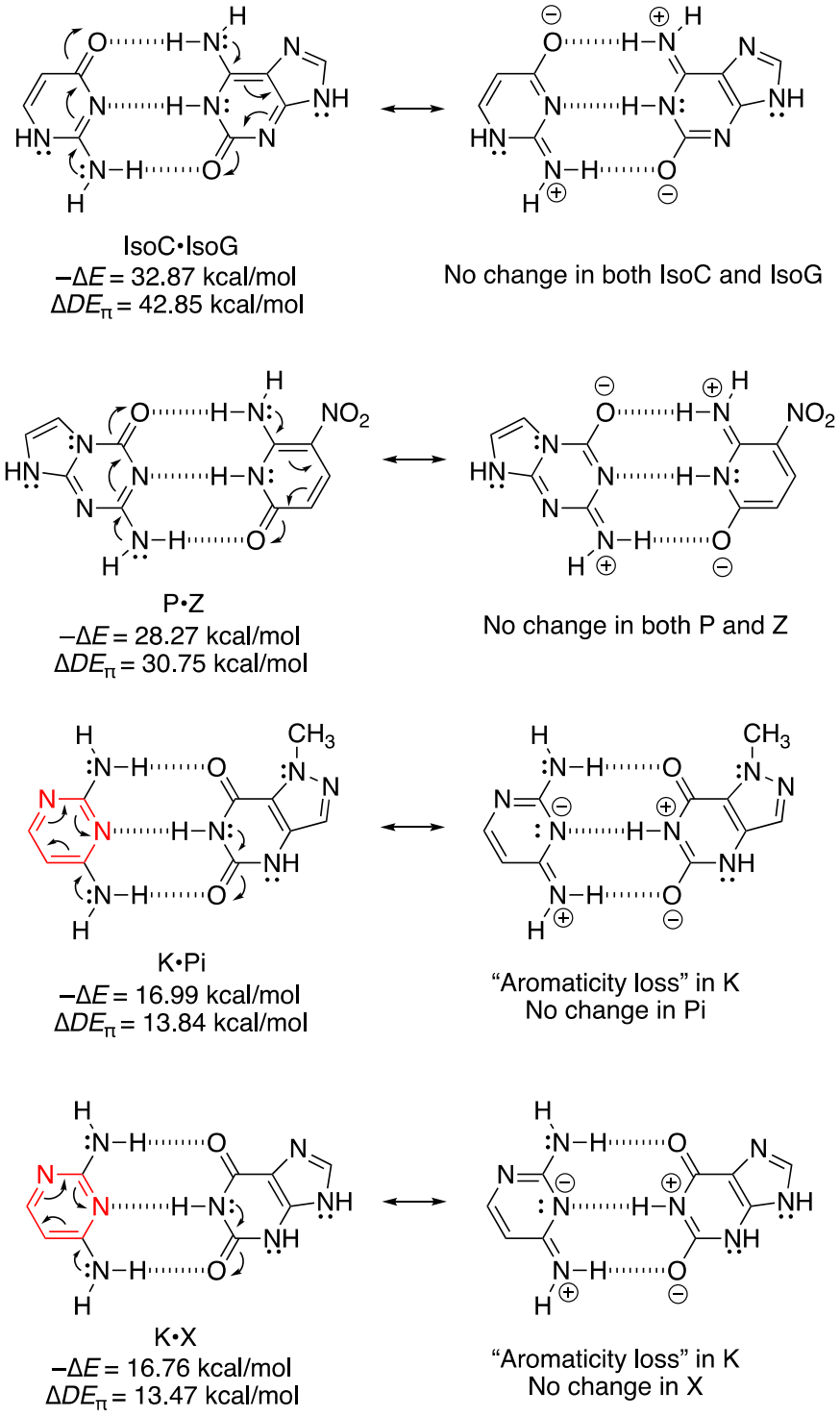
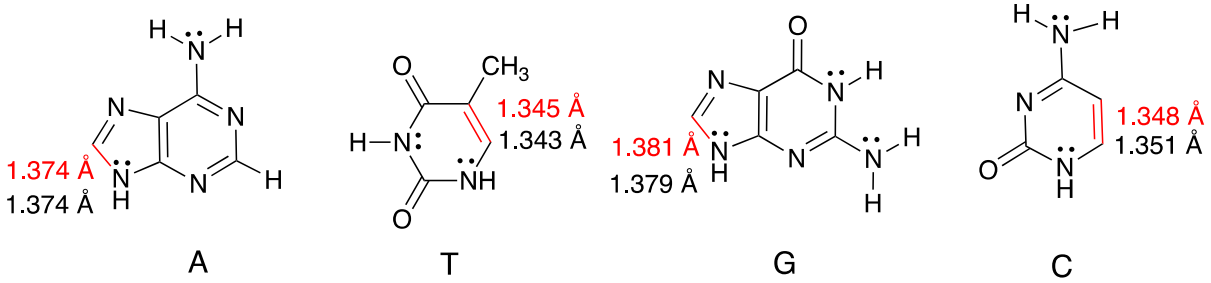


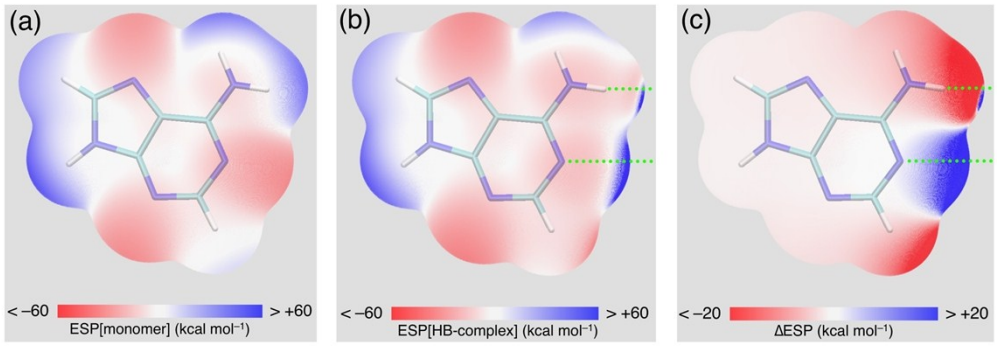
Figure S3. Resonance forms for base pairs shown in Figure 5 of the main text.

Electrostatic potential difference (ΔESP) plots.
Electrostatic potential (ESP) values for the isolated and the paired A, T, G, C bases were computed using their optimized geometries at C_s (see Geometric constrains, below), and differences of the computed ESP values were taken to generate the ΔESP plots. The computed ΔESP plots provide a measure of the change in electrostatic potential of A, T, G, C upon hydrogen bonding to form A•T and G•C (see Figure 3 in the main text and Figure S4). Positive ΔESP values (blue color) indicate a more repulsive surface, and negative ΔESP values (red color) indicate a more attractive surface upon base pairing.

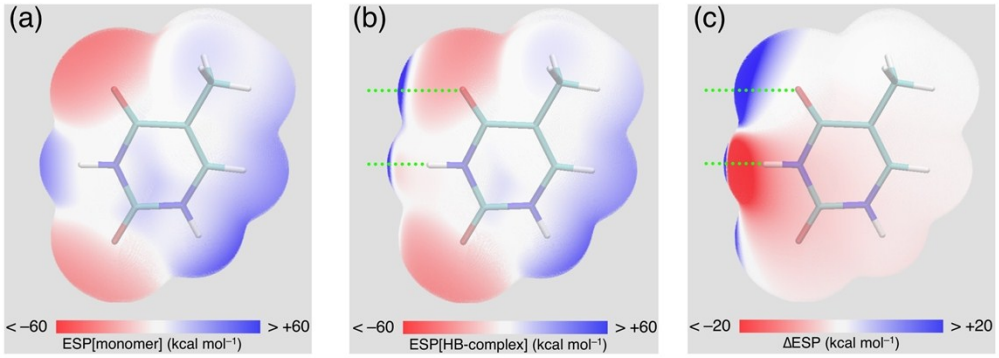
Generating the electron density isosurface. For a given base, ESP values for the isolated and paired states were computed using a common isosurface, constructed based on the geometry of the isolated base (see Geometric constraints, below), using an electron density isosurface of $\rho = 0.001$ e au^{-3} and a 0.05 bohr grid. For example, the change in electrostatic potential of guanine upon base pairing to form G•C was evaluated by: $\Delta ESP_G[G] = ESP_G[G•C\ pair] - ESP_G[G]$. Subscript "G" indicates that the isosurface used for computing the ESP values of guanine, in both the isolated and hydrogen-bonded states, were constructed based on the optimized geometry of isolated guanine. Isosurface coordinates were generated using MultiWFN program, followed by input to the Gaussian 09 program to compute the ESP values. All computations were performed at the ωB97X-D/6-311+G(d,p) level.

Geometric constraints. To ensure a consistent Cartesian framework for comparing the computed ESP values for a given base, in its isolated and paired state, selected ring bonds were fixed to the optimized geometry of A•T and G•C at C_s symmetry, so that the structures of the complex and monomer could be superimposed at these sites, followed by generation of the ΔESP plots. As shown below, the bonds colored in red were fixed to the values shown in red. The values in black are computed bond distances based on geometry optimizations of the isolated A, T, G, and C. The computed energy difference between the reference structure below and optimized C_s structures of A, T, G, and C are negligible (< 0.005 kcal/mol).

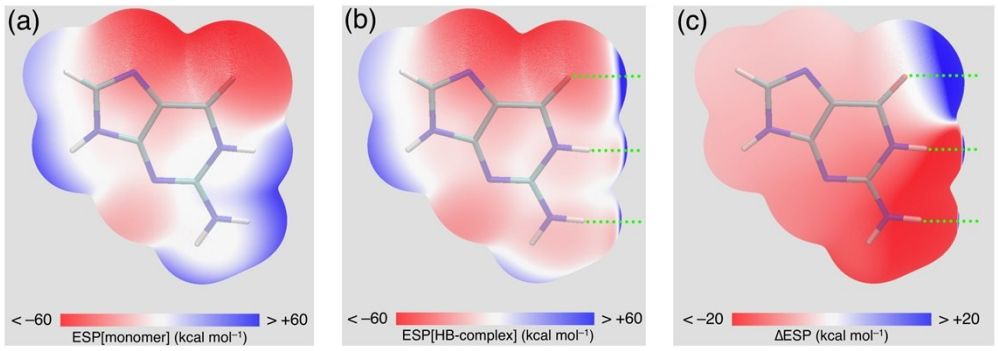




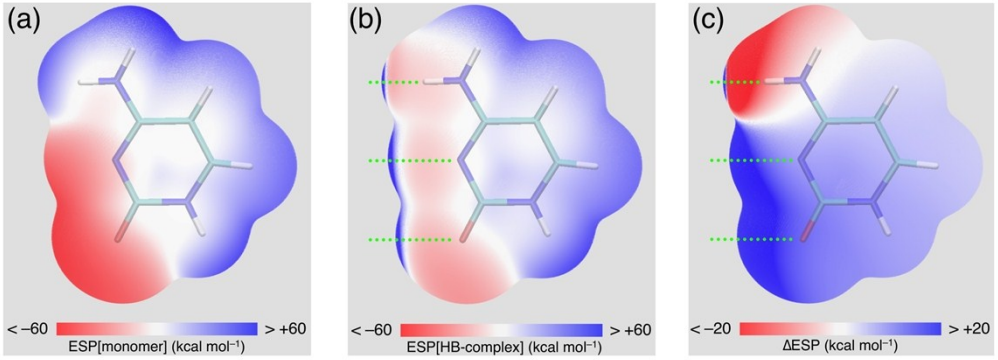
ESP plot of a) the adenine (A) monomer, b) adenine paired in A•T, and the c) ΔESP plot.



ESP plot of a) the thymine (T) monomer, b) thymine paired in A•T, and the c) ΔESP plot.



ESP plot of a) the guanine (G) monomer, b) guanine paired in G•C, and the c) ΔESP plot.



ESP plot of a) the cytosine (C) monomer, b) cytosine paired in G•C, and the c) ΔESP plot.

Figure S4. ESP and ΔESP plots for A, T, G, C upon base pairing to form A•T and G•C.

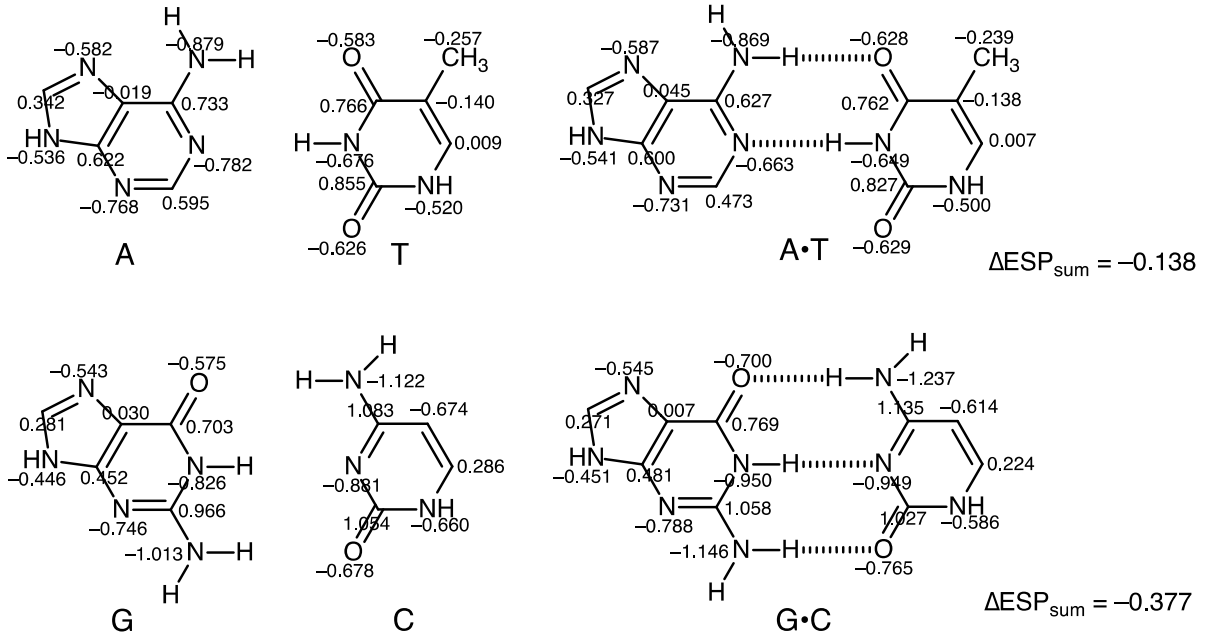
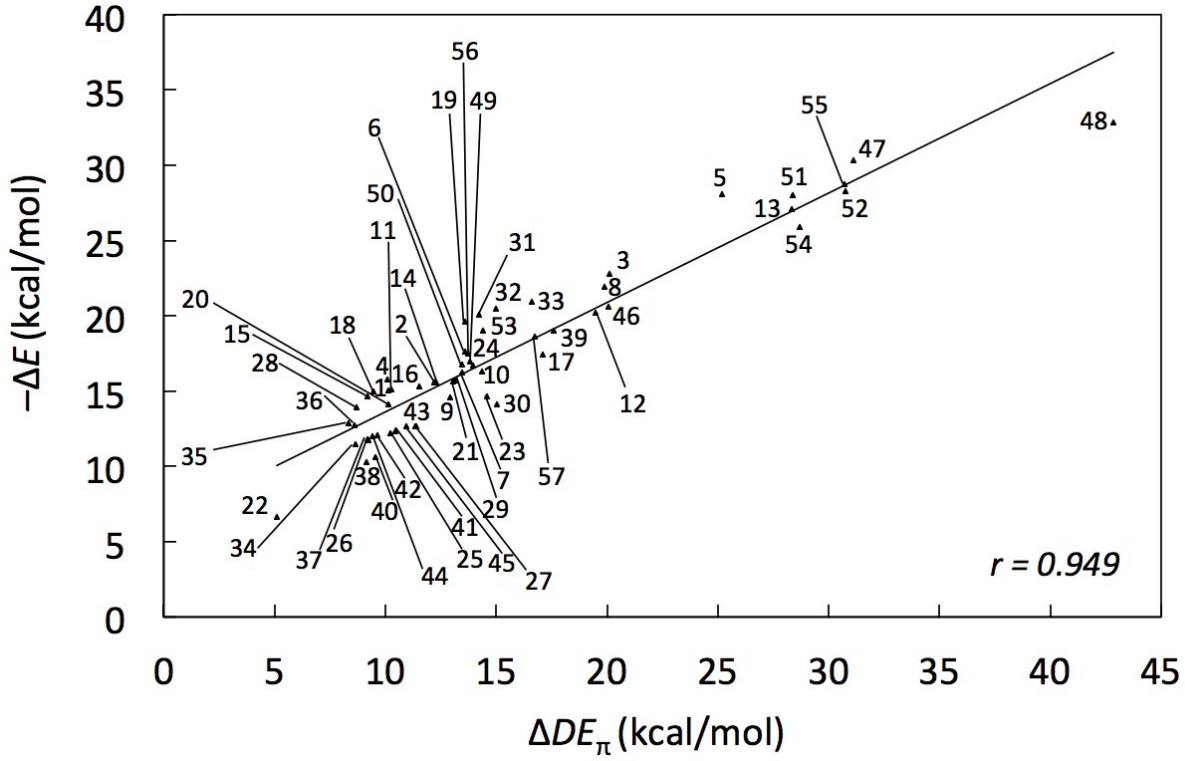


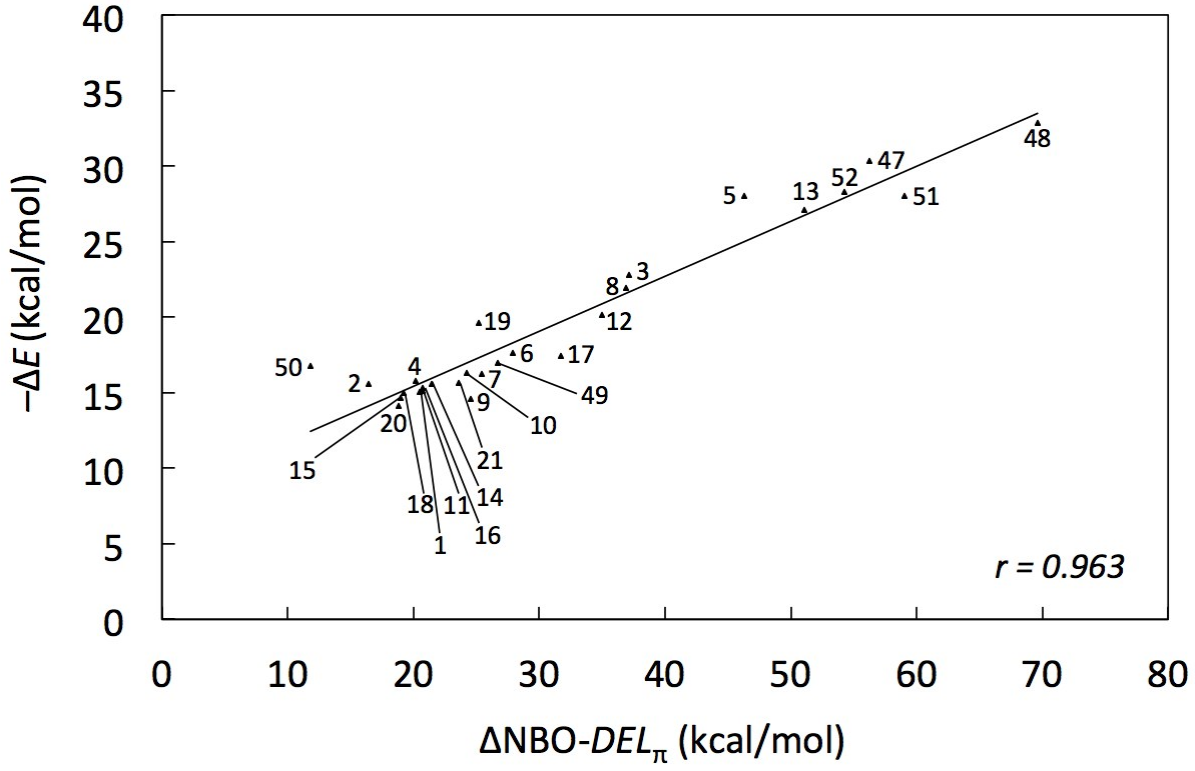
Figure S5. ESP-derived charges for A, T, G, C and the A•T, G•C pairs at a constrained C_s symmetry using the pop=chelpg keyword. Note the much larger change in charge distribution of G and C (upon pairing to form G•C) indicating the greater polarizability of these bases.



Label:

1. A•T	16. Reverse A•U(Hoog)	31. G•G 3	46. I•I
2. A•T(Hoog)	17. Reverse G•U	32. G•6-thioG 3	47. G•yC
3. A_{imino}•C	18. A•yT	33. 6-thioG•G 3	48. IsoC•IsoG
4. A•C_{imino}	19. T(h)•G	34. G•A 2	49. K•Pi
5. A_{imino}•T_{enol}	20. Reverse G•C	35. G•A 4	50. K•X
6. A_{imino}•T	21. Reverse A•C	36. A•A 1	51. G•C
7. I•A	22. G•A_{imino}	37. A•A 2	52. P•Z
8. I•C	23. Syn-G•A	38. A•A 3	53. G*•T
9. I•U	24. G•A	39. 8-oxoG•G	54. 6-thioG•C
10. G•U	25. U•U 1	40. 2-thioU•2-thioU	55. 8-oxoG•C
11. A•U	26. U•U 2	41. T•T 1	56. 2-aminoA•T
12. C•C	27. U•U 3	42. T•T 2	57. A•T(Hoog')
13. G•G	28. A•4-thioU	43. T•T 3	
14. 8-oxoG•A	29. G•4-thioU	44. T•C 1	
15. Reverse A•U	30. G•2-thioU	45. T•C 2	

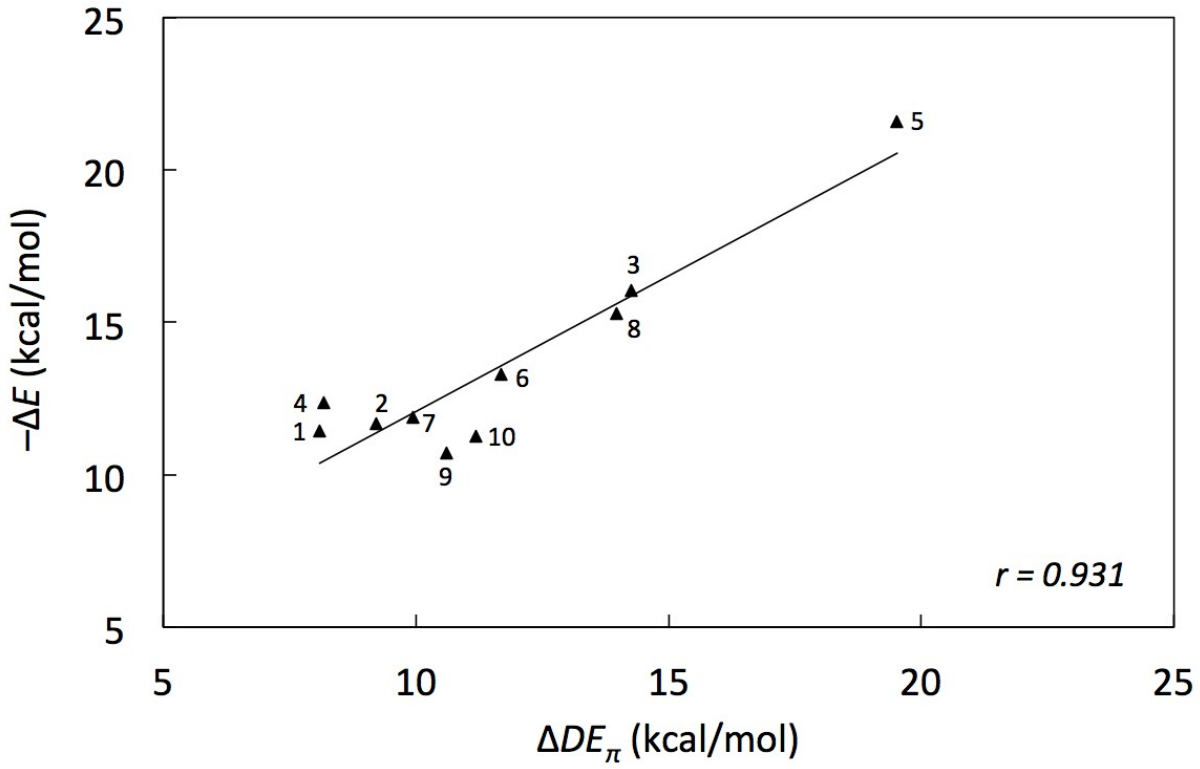
Figure S6. Plot of $-\Delta E$ vs. ΔDE_π for all nucleobase pairs. All geometries were optimized in the gas-phase with a constrained C_s symmetry at the ωB97X-D/6-311+G(d,p) level. BLW computations were performed at B3LYP/6-31G(d).



Label:

1. A•T	8. I•C	15. Reverse A•U	47. G•yC
2. A•T(Hoog)	9. I•U	16. Reverse A•U(Hoog)	48. IsoC•IsoG
3. A_{imino}•C	10. G•U	17. Reverse G•U	49. K•Pi
4. A•C_{imino}	11. A•U	18. A•yT	50. K•X
5. A_{imino}•T_{enol}	12. C•C	19. T(h)•G	51. G•C
6. A_{imino}•T	13. G•G	20. Reverse G•C	52. P•Z
7. I•A	14. 8-oxoG•A	21. Reverse A•C	

Figure S7. Plot of $-\Delta E$ vs. ΔNBO-DEL_π for selected nucleobase pairs in the gas-phase. All geometries were optimized with a constrained C_s symmetry at the ωB97X-D/6-311+G(d,p) level. NBO deletion computations were performed at ωB97X-D/def2-TZVPP.



Label:

1. A•T	4. A•C_{imino}	7. I•A	10. G•U
2. A•T(Hoog)	5. A_{imino}•T_{enol}	8. I•C	
3. A_{imino}•C	6. A_{imino}•T	9. I•U	

Figure S8. Plot of $-\Delta E$ vs. ΔDE_{π} for selected nucleobase pairs in chloroform. All geometries were optimized with a constrained C_s symmetry at the IEF-PCM-ωB97X-D/6-311+G(d,p) level. BLW computations were performed at B3LYP/6-31G(d).

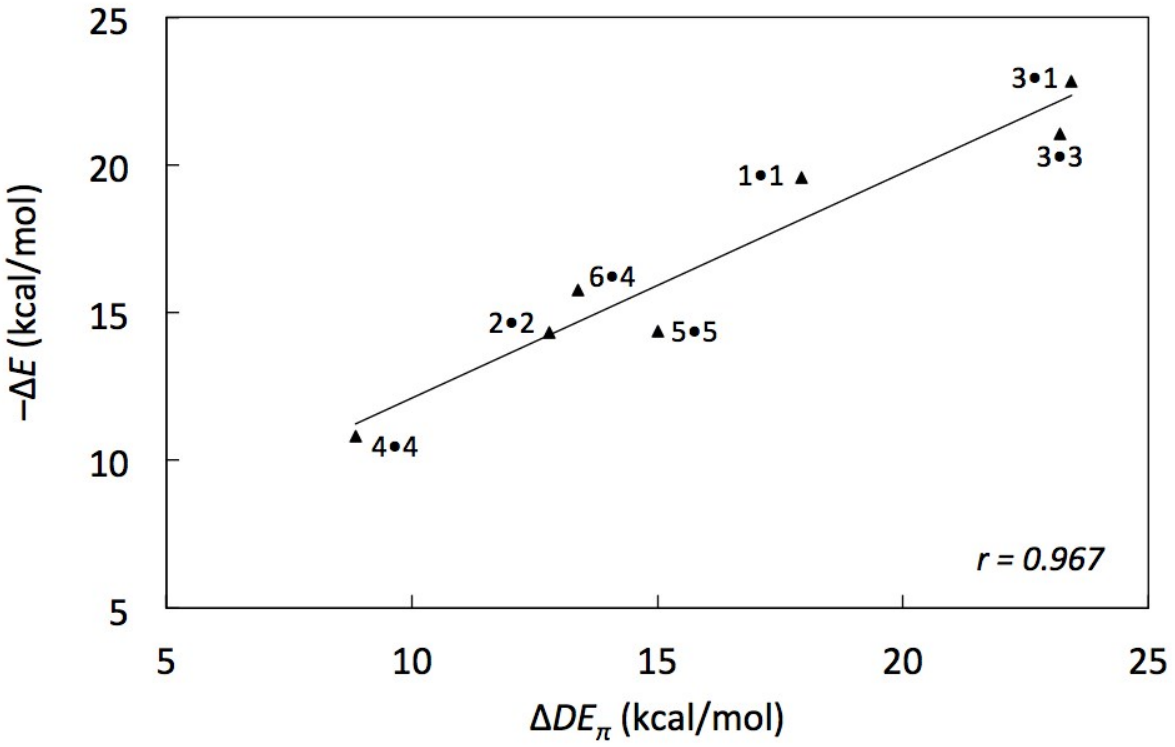


Figure S9. Plot of $-\Delta E$ vs. ΔDE_π for acyclic references. All geometries were optimized in the gas-phase with a constrained C_s symmetry at the ωB97X-D/6-311+G(d,p) level. BLW computations were performed at B3LYP/6-31G(d).

Table S1. Computed DE_{π}, ΔDE_{π}, and $-\Delta E$ values for all nucleobase pairs (A•B) and their monomers (A and B) in the gas-phase. All structures were optimized with a constrained C_s symmetry at ωB97X-D/6-311+G(d,p), and negative values of the computed interaction energies ($-\Delta E$) include ZPE correction. BLW computations were performed at the B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(A\bullet B)} - [DE_{\pi(A)} + DE_{\pi(B)}]$. All values are in kcal/mol.

A•B	$DE_{\pi(A\bullet B)}$	$DE_{\pi(A)}$	$DE_{\pi(B)}$	ΔDE_{π}	$-\Delta E$
A•T	326.03	201.91	113.97	10.15	15.06
A•T(Hoog)	328.06	201.91	113.97	12.18	15.58
A_{imino}•C	312.25	171.79	120.33	20.12	22.79
A•C_{imino}	317.18	201.91	105.19	10.09	15.79
A_{imino}•T_{enol}	316.07	171.79	119.08	25.19	28.05
A_{imino}•T	299.37	171.79	113.97	13.61	17.66
I•A	390.98	175.61	201.91	13.47	16.25
I•C	315.83	175.61	120.33	19.89	21.96
I•U	296.18	175.61	107.66	12.92	14.60
G•U	320.30	197.99	107.66	14.36	16.32
A•U	319.93	201.94	107.73	10.26	15.14
C•C	260.20	120.36	120.36	19.48	20.18
G•G	424.57	198.12	198.12	28.33	27.10
8-oxoG•A	433.63	219.41	201.94	12.28	15.58
r-A•U[1]	318.86	201.94	107.73	9.19	14.67
r-A•U(Hoog)	321.19	201.94	107.73	11.52	15.31
r-G•U	322.97	198.12	107.73	17.12	17.43
A•yT	401.81	201.94	190.43	9.44	14.96
T(h)•G	385.01	155.30	215.86	13.58	19.64
r-G•C	328.61	198.12	120.36	10.13	14.11
r-A•C	335.36	201.94	120.36	13.06	15.62
G•A_{imino}	375.05	198.12	171.82	5.11	6.62
Syn-G•A	414.65	198.12	201.94	14.59	14.65
G•A	414.01	198.12	201.94	13.95	16.73
U•U 1	225.67	107.73	107.73	10.22	12.18
U•U 2	224.70	107.73	107.73	9.25	11.73
U•U 3	226.87	107.73	107.73	11.41	12.68
A•4-thioU	329.58	201.94	118.95	8.69	13.92
G•4-thioU	330.21	198.12	118.95	13.14	15.69
G•2-thioU	334.13	198.12	120.96	15.04	14.14
G•G 3	410.45	198.12	198.12	14.20	20.08
G•6-thioG 3	425.08	198.12	211.95	15.01	20.49
6-thioG•G 3	426.70	211.95	198.12	16.63	20.97
G•A 2	408.70	198.12	201.94	8.63	11.46
G•A 4	408.41	198.12	201.94	8.34	12.84
A•A 1	412.48	201.94	201.94	8.60	12.76
A•A 2	413.09	201.94	201.94	9.20	11.82
A•A 3	413.05	201.94	201.94	9.16	10.26
8oxoG•G	435.11	219.41	198.12	17.59	19.01
2-thioU•2-thioU	251.45	120.96	120.96	9.53	10.61

T•T 1	238.39	113.96	113.96	10.47	12.37
T•T 2	237.57	113.96	113.96	9.65	12.07
T•T 3	239.29	113.96	113.96	11.36	12.69
T•C 1	243.73	113.96	120.36	9.41	12.03
T•C 2	245.29	113.96	120.36	10.97	12.64
I•I	371.29	175.62	175.62	20.06	20.63
A•T(Hoog')	332.63	201.94	113.96	16.73	18.62
G•yC	419.25	198.12	190.01	31.12	30.36
IsoC•IsoG	344.10	195.97	105.28	42.85	32.87
K•Pi	357.74	195.97	113.96	13.84	16.99
K•X	307.49	95.79	198.12	13.47	16.76
G•C	346.83	198.11	120.36	28.37	28.05
P•Z	456.64	203.98	221.91	30.75	28.27
G*•T	348.29	219.91	113.96	14.42	18.99
6-thioG•C	360.99	211.95	120.36	28.68	25.88
8-oxoG•C	370.47	219.41	120.36	30.70	28.75
2-aminoA•T	352.14	224.43	113.96	13.75	17.51

(1) "r": the base pair adopts a reverse structure.

Table S2. Computed NBO–DEL_{π}, ΔNBO–DEL_{π}, and –ΔE values for selected nucleobase pairs (A•B) and their monomers (A and B) in the gas-phase. All structures were optimized with C_s symmetry. NBO deletion computations were performed at the ωB97X-D/def2-TZVPP level; $\Delta DEL_{\pi} = DEL_{\pi(A\bullet B)} - [DEL_{\pi(A)} + DEL_{\pi(B)}]$. Negative values of the interaction energies with ZPE correction (–ΔE) were computed at ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

A•B	$DEL_{\pi(A\bullet B)}$	$DEL_{\pi(A)}$	$DEL_{\pi(B)}$	ΔDEL_{π}	$-\Delta E$
A•T	542.15	314.17	207.46	20.52	15.06
A•T(Hoog)	543.40	314.17	212.79	16.43	15.58
A_{imino}•C	524.97	279.01	208.83	37.13	22.79
A•C_{imino}	528.17	314.17	193.80	20.20	15.79
A_{imino}•T_{enol}	528.62	279.01	203.32	46.30	28.05
A_{imino}•T	514.38	279.01	207.46	27.91	17.66
I•A	625.93	286.32	314.17	25.44	16.25
I•C	532.03	286.32	208.83	36.88	21.96
I•U	511.32	286.32	200.42	24.58	14.60
G•U	558.99	334.30	200.42	24.27	16.32
A•U	535.34	314.17	200.42	20.74	15.14
C•C	452.63	208.83	208.83	34.97	20.18
G•G	713.68	331.32	331.32	51.04	27.10
8-oxoG•A	716.02	380.44	314.17	21.42	15.58
r-A•U	533.61	314.17	200.42	19.01	14.67
r-A•U(Hoog)	535.32	314.17	200.42	20.73	15.31
r-G•U	563.47	331.32	200.42	31.73	17.43
A•yT	653.33	314.17	319.91	19.24	14.96
G•yC	695.16	331.32	307.56	56.28	30.36
IsoC•IsoG	596.82	342.79	184.42	69.61	32.87
K•Pi	621.96	250.47	344.80	26.69	16.99
T(h)•G	515.57	159.04	331.32	25.21	19.64
K•X	584.89	322.61	250.47	11.81	16.76
G•C	608.90	341.07	208.83	59.00	28.05
r-G•C	558.95	331.32	208.83	18.80	14.11
r-A•C	546.64	314.17	208.83	23.64	15.62
P•Z	776.66	350.26	372.14	54.27	28.27

Table S3. Computed DE_{π}, ΔDE_{π}, and $-\Delta E$ values for all nucleobase pairs (A•B) and their monomers (A and B) in chloroform. All structures were optimized with a constrained C_s symmetry at the IEF-PCM-ωB97X-D/6-311+G(d,p), and negative values of the computed interaction energies ($-\Delta E$) include ZPE correction. BLW computations were performed at the B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(A\bullet B)} - [DE_{\pi(A)} + DE_{\pi(B)}]$. All values are in kcal/mol.

A•B	$DE_{\pi(A\bullet B)}$	$DE_{\pi(A)}$	$DE_{\pi(B)}$	ΔDE_{π}	$-\Delta E$
A•T	331.17	204.41	118.67	8.09	11.45
A•T(Hoog)	332.30	204.41	118.67	9.22	11.67
A_{imino}•C	317.07	175.26	127.56	14.25	16.06
A•C_{imino}	321.00	204.41	108.43	8.16	12.35
A_{imino}•T_{enol}	319.83	175.26	125.06	19.52	21.60
A_{imino}•T	305.62	175.26	118.67	11.69	13.30
I•A	395.27	180.91	204.41	9.95	11.87
I•C	322.44	180.91	127.56	13.97	15.29
I•U	304.17	180.91	112.66	10.60	10.71
G•U	329.78	205.94	112.66	11.18	11.25

Table S4. Computed DE_{π}, ΔDE_{π}, and $-\Delta E$ values for all acyclic references (A•B) and their monomers (A and B) in the gas-phase. All structures were optimized with a constrained C_s symmetry at ωB97X-D/6-311+G(d,p), and negative values of the computed interaction energies ($-\Delta E$) include ZPE correction. BLW computations were performed at the B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(A\bullet B)} - [DE_{\pi(A)} + DE_{\pi(B)}]$. All values are in kcal/mol.

A•B	$DE_{\pi(A\bullet B)}$	$DE_{\pi(A)}$	$DE_{\pi(B)}$	ΔDE_{π}	$-\Delta E$
1•1	150.09	66.08	66.08	17.94	19.57
2•2	107.41	47.31	47.31	12.79	14.32
3•3	129.11	52.95	52.95	23.20	21.07
4•4	111.20	51.18	51.18	8.85	10.80
5•5	103.55	44.27	44.27	15.00	14.39
3•1	142.47	52.95	66.08	23.44	22.85
6•4	130.37	65.81	51.18	13.39	15.78

Table S5. Computed planarization energies (C_1 minima vs. planar C_s) for nucleobases and base pairs with a nonplanar minima at ωB97X-D/6-311+G(d,p) (without ZPE correction). All values are in kcal/mol.

	ΔE
C	–0.004
G	–0.42
8-oxoG	–0.34
yC	–0.47
IsoG	–0.02
IsoC	–0.62
K	–0.17
Pi	–0.10
G*	–0.10
6-thioG	–0.32
2-aminoA	–0.15
1	–4.67
2	–0.19
5	–3.22
6	–3.47
G•U	–0.06
8-oxoG•A	–0.42
r-G•U	–0.08
K•Pi	–0.11
r-G•C	–4.70
G•A$_{imino}$	–0.23
Syn-G•A	–2.11
G•A	–1.02
G•4-thioU	–0.07
G•2-thioU	–0.21
G•G 3	–0.31
G•6-thioG 3	–0.23
6-thioG•G 3	–0.31
G•A 2	–0.84
G•A 4	–0.10
8-oxoG•G	–0.41
1•1	–3.47
2•2	–0.45
5•5	–4.89
3•1	–1.34
6•4	–3.41

Table S6. Optimized Cartesian coordinates (in Å) and computed total electronic energies (including zero-point energies corrections) (in a.u.) for all structures at ωB97XD/6-311+G(d,p) in the gas-phase. All the geometries were optimized with a constrained C_s symmetry.

1. Nucleobases

A

	X	Y	Z
C	–2.29890	0.00005	0.00000
N	–1.14777	0.68352	0.00000
C	0.00041	–0.00024	0.00000
C	–0.05058	–1.40521	0.00000
N	–2.48250	–1.31421	0.00000
C	–1.31949	–1.96817	0.00000
N	–1.09680	–3.32166	0.00000
N	0.93114	–2.37665	0.00000
C	0.26614	–3.49607	0.00000
H	–1.80462	–4.03686	0.00000
N	1.16697	0.67496	0.00000
H	0.70825	–4.48176	0.00000
H	–3.19865	0.60784	0.00000
H	2.03953	0.17759	0.00000
H	1.14976	1.67938	0.00000

Sum of electronic and zero–point Energies: –467.175391 a.u.
N_{Im}= 0

T

	X	Y	Z
N	0.00808	1.37706	0.00000
C	–1.13647	2.14954	0.00000
N	–2.29180	1.39418	0.00000
C	–2.40899	–0.00010	0.00000
C	–1.13233	–0.72162	0.00000
C	0.00041	0.00000	0.00000
O	–1.12159	3.35802	0.00000
O	–3.50153	–0.52327	0.00000
C	–1.17280	–2.21764	0.00000
H	0.97948	–0.46402	0.00000
H	0.87431	1.89020	0.00000
H	–3.15694	1.91687	0.00000
H	–0.16479	–2.63688	0.00000
H	–1.70754	–2.58864	0.87767
H	–1.70754	–2.58864	–0.87767

Sum of electronic and zero–point Energies: –454.006104 a.u.
N_{Im}= 0

A_{imino}

	X	Y	Z
C	0.00000	0.00015	0.00000

N	1.20366	0.63039	0.00000
C	2.46888	–0.00017	0.00000
C	2.28722	–1.43422	0.00000
N	–0.17577	–1.28168	0.00000
C	1.01238	–1.95407	0.00000
N	1.18050	–3.31008	0.00000
N	3.22776	–2.43210	0.00000
C	2.53252	–3.53724	0.00000
H	0.44304	–3.99520	0.00000
N	3.50949	0.73067	0.00000
H	2.94268	–4.53585	0.00000
H	–0.86616	0.65386	0.00000
H	4.34031	0.14512	0.00000
H	1.23499	1.63988	0.00000

Sum of electronic and zero–point Energies: –467.155310 a.u.
N_{Im}= 0

C

	X	Y	Z
C	–0.08337	–1.41602	0.00000
N	1.10497	–2.09173	0.00000
C	2.24040	–1.43520	0.00000
C	2.34044	0.00039	0.00000
C	1.17035	0.67501	0.00000
N	0.00015	–0.00024	0.00000
O	–1.18123	–1.92722	0.00000
N	3.37700	–2.16944	0.00000
H	–0.88476	0.48233	0.00000
H	1.11149	1.75661	0.00000
H	3.29074	0.51418	0.00000
H	4.28524	–1.74454	0.00000
H	3.29292	–3.17170	0.00000

Sum of electronic and zero–point Energies: –394.816334 a.u.
N_{Im}= 1 (55*i* cm^{-1})

C_{imino}

	X	Y	Z
C	–0.10975	–1.38365	0.00000
N	1.10122	–2.02992	0.00000
C	2.38062	–1.45953	0.00000
C	2.37148	–0.00004	0.00000
C	1.20543	0.65975	0.00000
N	–0.00013	0.00006	0.00000
O	–1.17826	–1.94943	0.00000
N	3.37744	–2.25316	0.00000
H	–0.87303	0.50095	0.00000
H	1.14614	1.74066	0.00000
H	3.31089	0.53337	0.00000
H	4.24978	–1.73346	0.00000
H	1.06110	–3.03935	0.00000

Sum of electronic and zero–point Energies: –394.812888 a.u.
N_{Im}= 0

T_{enol}

	X	Y	Z
N	1.13228	1.98425	0.00000
C	–0.10253	1.30751	0.00000
N	–0.01816	–0.06612	0.00000
C	1.14280	–0.64529	0.00000
C	2.42021	0.00795	0.00000
C	2.33631	1.35897	0.00000
O	–1.13207	1.94158	0.00000
O	1.17277	–1.98049	0.00000
C	3.70745	–0.75974	0.00000
H	3.21203	1.99760	0.00000
H	1.07099	2.99065	0.00000
H	4.56049	–0.07808	0.00000
H	3.78228	–1.40354	0.87975
H	3.78228	–1.40354	–0.87975
H	0.25447	–2.27786	0.00000

Sum of electronic and zero–point Energies: –453.984131 a.u.
N_{Im}= 0

I

	X	Y	Z
N	0.79598	1.38462	0.00000
C	1.41866	0.10320	0.00000
C	2.85137	0.27734	0.00000
C	3.37262	1.55988	0.00000
N	2.71081	2.74816	0.00000
C	1.42725	2.58959	0.00000
H	0.78175	3.46187	0.00000
O	0.74653	–0.89942	0.00000
N	3.85592	–0.65880	0.00000
C	4.95457	0.04030	0.00000
N	4.72654	1.39443	0.00000
H	–0.21413	1.35766	0.00000
H	5.40948	2.13407	0.00000
H	5.95497	–0.36635	0.00000

Sum of electronic and zero–point Energies: –487.054997 a.u.
N_{Im}= 0

U

	X	Y	Z
C	–2.46152	–1.40900	0.00000
O	–3.50214	–2.02117	0.00000
N	–2.37541	–0.03246	0.00000
C	–1.21767	0.76227	0.00000
C	0.01975	–0.00911	0.00000
N	–1.22272	–2.03165	0.00000

C	–0.03217	–1.34971	0.00000
H	–3.25807	0.46032	0.00000
O	–1.30393	1.96848	0.00000
H	0.95624	0.52708	0.00000
H	–1.24796	–3.03840	0.00000
H	0.85649	–1.96816	0.00000

Sum of electronic and zero–point Energies: –414.716018 a.u.
N_{Im}= 0

G

	X	Y	Z
N	–3.56382	–0.99855	0.00000
C	–2.56051	0.01921	0.00000
C	–1.25907	–0.58860	0.00000
C	–1.17217	–1.97063	0.00000
N	–2.16501	–2.89255	0.00000
C	–3.35126	–2.34953	0.00000
N	–4.44929	–3.14876	0.00000
O	–2.89791	1.17935	0.00000
N	–0.00592	–0.01663	0.00000
C	0.81355	–1.02412	0.00000
N	0.16382	–2.24050	0.00000
H	–4.50508	–0.63227	0.00000
H	–5.38475	–2.78878	0.00000
H	–4.30139	–4.14178	0.00000
H	0.57650	–3.15824	0.00000
H	1.89137	–0.95830	0.00000

Sum of electronic and zero–point Energies: –542.410714 a.u.
N_{Im}= 1 (327*i* cm^{-1})

8-oxoG

	X	Y	Z
C	3.64565	0.33262	0.00000
C	2.27028	0.00227	0.00000
N	1.12553	0.79484	0.00000
C	–0.00311	0.00479	0.00000
N	0.49626	–1.30698	0.00000
C	1.86565	–1.30880	0.00000
N	2.64850	–2.40657	0.00000
C	3.92817	–2.13264	0.00000
N	4.42286	–0.86090	0.00000
N	4.82230	–3.15250	0.00000
O	–1.16440	0.33844	0.00000
H	1.09606	1.79928	0.00000
H	5.41952	–0.69658	0.00000
O	4.19159	1.41961	0.00000
H	–0.09921	–2.11750	0.00000
H	5.81436	–3.00805	0.00000
H	4.45890	–4.08869	0.00000

Sum of electronic and zero–point Energies: –617.662717 a.u.

N_{Im}= 1 (312*i* cm^{-1})

yT

	X	Y	Z
C	–1.81581	1.77946	0.00000
N	–2.45054	0.54691	0.00000
C	–1.86970	–0.71744	0.00000
C	–0.39499	–0.70185	0.00000
N	–0.44290	1.70018	0.00000
C	0.28485	0.51899	0.00000
O	–2.41837	2.82669	0.00000
H	–3.46065	0.58062	0.00000
O	–2.55315	–1.71495	0.00000
C	1.68143	0.53632	0.00000
H	0.03274	2.58865	0.00000
H	2.21125	1.48260	0.00000
C	2.37673	–0.65952	0.00000
H	3.46065	–0.64021	0.00000
C	1.70374	–1.88325	0.00000
H	2.26146	–2.81140	0.00000
C	0.32200	–1.89850	0.00000
H	–0.23711	–2.82669	0.00000

Sum of electronic and zero–point Energies: –568.304949 a.u.
N_{Im}= 0

yC

	X	Y	Z
C	0.07353	1.16765	0.00000
N	0.01442	–0.12665	0.00000
C	1.18008	–0.87577	0.00000
O	1.15922	–2.08853	0.00000
C	2.47306	–0.12903	0.00000
C	2.46455	1.26442	0.00000
N	1.22818	1.90075	0.00000
N	–1.08539	1.87548	0.00000
C	3.65692	1.98954	0.00000
H	1.19713	2.90663	0.00000
H	–1.93827	1.34436	0.00000
H	–1.12380	2.87741	0.00000
H	3.63840	3.07466	0.00000
C	4.85930	1.30480	0.00000
H	5.78852	1.86326	0.00000
C	4.88484	–0.09151	0.00000
H	5.83284	–0.61581	0.00000
C	3.69618	–0.79909	0.00000
H	3.67644	–1.88260	0.00000

Sum of electronic and zero–point Energies: –548.390209 a.u.
N_{Im}= 1 (324*i* cm^{-1})

IsoG

	X	Y	Z
C	0.94177	0.84402	0.00000
C	–0.22768	0.10623	0.00000
C	–0.09065	–1.29263	0.00000
N	0.99606	–2.03288	0.00000
C	2.16348	–1.34114	0.00000
N	2.07423	0.10902	0.00000
N	0.98213	2.18817	0.00000
O	3.28516	–1.79974	0.00000
N	–1.55719	0.49711	0.00000
C	–2.20903	–0.62264	0.00000
N	–1.38936	–1.73555	0.00000
H	–3.28516	–0.71656	0.00000
H	–1.66931	–2.70231	0.00000
H	1.84408	2.70231	0.00000
H	0.11063	2.69051	0.00000
H	2.98067	0.55373	0.00000

Sum of electronic and zero–point Energies: –542.403977 a.u.
N_{Im}= 1 (132*i* cm^{-1})

IsoC

	X	Y	Z
C	0.03440	1.24120	0.00000
N	0.03459	–0.15460	0.00000
C	1.15116	–0.80331	0.00000
N	1.13725	–2.16332	0.00000
N	2.38884	–0.20762	0.00000
C	2.46962	1.17090	0.00000
C	1.35213	1.90500	0.00000
O	–1.00057	1.87491	0.00000
H	3.22893	–0.75969	0.00000
H	3.47042	1.58319	0.00000
H	1.38627	2.98513	0.00000
H	1.96610	–2.72725	0.00000
H	0.23532	–2.60584	0.00000

Sum of electronic and zero–point Energies: –394.800066 a.u.
N_{Im}= 1 (354*i* cm^{-1})

K

	X	Y	Z
C	0.16426	1.22179	0.00000
N	0.08849	–0.11483	0.00000
C	1.24398	–0.77620	0.00000
N	1.16608	–2.13207	0.00000
C	2.48070	–0.10416	0.00000
C	2.41577	1.27191	0.00000
N	1.27713	1.96565	0.00000
N	–1.01532	1.89185	0.00000
H	1.98878	–2.70462	0.00000
H	0.25830	–2.56185	0.00000

H	–1.00633	2.89485	0.00000
H	–1.87703	1.37905	0.00000
H	3.32888	1.86159	0.00000
H	3.42424	–0.63336	0.00000

Sum of electronic and zero–point Energies: –374.938012 a.u.
N_{Im}= 2 (226*i* cm^{-1}, 198*i* cm^{-1})

Pi

	X	Y	Z
C	0.92322	1.20747	0.00000
C	–0.28338	0.40726	0.00000
C	–0.26223	–0.97157	0.00000
N	0.93593	–1.65856	0.00000
C	2.14755	–1.00550	0.00000
N	2.05538	0.38882	0.00000
O	1.00309	2.41571	0.00000
O	3.21205	–1.57717	0.00000
N	–1.58979	0.77948	0.00000
N	–2.38944	–0.27642	0.00000
C	–1.60967	–1.35804	0.00000
H	2.94716	0.86461	0.00000
H	0.97756	–2.66435	0.00000
C	–2.12843	2.12753	0.00000
H	–3.21205	2.03443	0.00000
H	–1.79250	2.66435	0.88711
H	–1.79250	2.66435	–0.88711
H	–2.04692	–2.34383	0.00000

Sum of electronic and zero–point Energies: –601.567341 a.u.
N_{Im}= 1 (93*i* cm^{-1})

T(h)

	X	Y	Z
C	0.09477	1.01820	0.00000
N	0.12574	–0.27906	0.00000
C	1.35180	–0.92745	0.00000
N	2.48059	–0.08882	0.00000
C	2.42581	1.26590	0.00000
C	1.22453	1.89504	0.00000
H	3.36831	–0.56866	0.00000
H	3.37570	1.78874	0.00000
C	1.06209	3.38739	0.00000
H	2.03223	3.88846	0.00000
H	0.51203	3.72597	–0.88243
H	0.51203	3.72597	0.88243
O	1.49749	–2.12731	0.00000
H	–0.90007	1.46702	0.00000

Sum of electronic and zero–point Energies: –378.739722 a.u.
N_{Im}= 0

X

	X	Y	Z
N	–2.08795	–0.00241	0.00000
C	–1.44386	–1.26676	0.00000
C	–0.00096	–1.11252	0.00000
C	0.54898	0.14326	0.00000
N	–0.16559	1.31000	0.00000
C	–1.55598	1.27298	0.00000
O	–2.22369	2.27950	0.00000
O	–2.09462	–2.27950	0.00000
N	0.99220	–2.06627	0.00000
C	2.10250	–1.40001	0.00000
N	1.89574	–0.02804	0.00000
H	–3.09818	–0.03439	0.00000
H	2.60529	0.68550	0.00000
H	3.09818	–1.81650	0.00000
H	0.25278	2.22577	0.00000

Sum of electronic and zero–point Energies: –562.299005 a.u.
N_{Im}= 0

P

	X	Y	Z
N	2.11541	–0.09266	0.00000
C	1.56527	1.13943	0.00000
N	0.12111	1.12848	0.00000
C	–0.55944	–0.04372	0.00000
N	–0.01657	–1.23457	0.00000
C	1.34194	–1.17134	0.00000
N	1.96861	–2.36551	0.00000
O	2.12399	2.20955	0.00000
C	–0.77022	2.19515	0.00000
C	–2.00799	1.66648	0.00000
N	–1.87397	0.27862	0.00000
H	2.97234	–2.38544	0.00000
H	1.42898	–3.21135	0.00000
H	–2.61115	–0.40472	0.00000
H	–2.97234	2.14300	0.00000
H	–0.41793	3.21135	0.00000

Sum of electronic and zero–point Energies: –542.410959 a.u.
N_{Im}= 0

Z

	X	Y	Z
N	–0.60466	–1.21469	0.00000
C	0.01688	–2.48908	0.00000
O	–0.68819	–3.47458	0.00000
C	1.45966	–2.43228	0.00000
C	2.09961	–1.24171	0.00000
C	1.40394	–0.00130	0.00000
C	0.00319	–0.00037	0.00000
N	–0.77802	1.08668	0.00000

N	2.15430	1.20962	0.00000
O	1.54634	2.28619	0.00000
O	3.36966	1.13995	0.00000
H	1.99007	–3.37367	0.00000
H	3.18117	–1.19313	0.00000
H	–0.31638	1.98686	0.00000
H	–1.77958	1.01091	0.00000
H	–1.61449	–1.26509	0.00000

Sum of electronic and zero–point Energies: –583.252360 a.u.
N_{Im}= 0

4-thioU

	X	Y	Z
C	–0.26162	1.06843	0.00000
N	–1.26865	0.12072	0.00000
C	–1.14052	–1.25721	0.00000
N	0.17681	–1.68161	0.00000
C	1.07094	0.51320	0.00000
C	1.24320	–0.82043	0.00000
S	–0.61170	2.68035	0.00000
H	–2.22104	0.46129	0.00000
O	–2.07955	–2.01415	0.00000
H	2.22104	–1.28452	0.00000
H	0.30856	–2.68035	0.00000
H	1.91235	1.18812	0.00000

Sum of electronic and zero–point Energies: –737.676642 a.u.
N_{Im}= 0

2-thioU

	X	Y	Z
C	–0.89306	–1.10341	0.00000
S	–1.86645	–2.44146	0.00000
N	–1.35933	0.17912	0.00000
C	–0.61312	1.37392	0.00000
C	0.82678	1.15816	0.00000
N	0.47527	–1.18683	0.00000
C	1.30600	–0.09513	0.00000
H	–2.36480	0.28762	0.00000
O	–1.17814	2.44146	0.00000
H	1.47553	2.02060	0.00000
H	0.85128	–2.12179	0.00000
H	2.36480	–0.32040	0.00000

Sum of electronic and zero–point Energies: –737.674154 a.u.
N_{Im}= 0

6-thioG

	X	Y	Z
C	0.32871	1.09109	0.00000
C	–0.77709	0.19945	0.00000
C	–0.53172	–1.16870	0.00000

N	0.65545	–1.81148	0.00000
C	1.66828	–0.98590	0.00000
N	1.53421	0.37486	0.00000
S	0.35580	2.74305	0.00000
N	2.93143	–1.47973	0.00000
N	–2.13237	0.44863	0.00000
C	–2.68321	–0.72577	0.00000
N	–1.76060	–1.75311	0.00000
H	3.04067	–2.47781	0.00000
H	3.74527	–0.89416	0.00000
H	–3.74527	–0.92134	0.00000
H	2.35630	0.96349	0.00000
H	–1.94173	–2.74305	0.00000

Sum of electronic and zero–point Energies: –865.373500 a.u.
N_{Im}= 1 (302*i* cm^{-1})

G*

	X	Y	Z
N	–3.61517	–0.97236	0.00000
C	–2.59802	–0.12994	0.00000
C	–1.28207	–0.60294	0.00000
C	–1.17124	–1.99425	0.00000
N	–2.15987	–2.88417	0.00000
C	–3.35766	–2.29961	0.00000
N	–4.44635	–3.10988	0.00000
O	–2.85946	1.17370	0.00000
N	–0.03534	–0.00308	0.00000
C	0.79505	–0.99926	0.00000
N	0.17461	–2.23339	0.00000
H	–5.36377	–2.70559	0.00000
H	–4.31922	–4.10469	0.00000
H	0.61220	–3.13916	0.00000
H	1.87190	–0.91276	0.00000
H	–3.81891	1.26598	0.00000

Sum of electronic and zero–point Energies: –542.408543 a.u.
N_{Im}= 1 (219*i* cm^{-1})

2-aminoA

	X	Y	Z
C	–0.64543	1.04264	0.00000
N	0.08693	–0.09114	0.00000
C	–0.55161	–1.25809	0.00000
C	–1.95855	–1.27249	0.00000
N	–1.97631	1.16217	0.00000
C	–2.57271	–0.02866	0.00000
N	–3.91424	–0.30845	0.00000
N	–2.88833	–2.29621	0.00000
C	–4.03428	–1.68280	0.00000
N	0.16849	–2.39863	0.00000
H	–5.00127	–2.16394	0.00000

N	0.07161	2.19732	0.00000
H	–0.29912	–3.28743	0.00000
H	1.17133	–2.34682	0.00000
H	–4.65784	0.36888	0.00000
H	–0.41069	3.07636	0.00000
H	1.07310	2.15361	0.00000

Sum of electronic and zero–point Energies: –522.535242 a.u.
N_{Im}= 1 (250*i* cm^{-1})

2. Nucleobase pairs

A•T

	X	Y	Z
C	–0.54905	0.94130	0.00000
C	3.63656	–1.27389	0.00000
N	0.12042	–0.22271	0.00000
N	2.94676	–0.07704	0.00000
C	–0.55787	–1.38343	0.00000
C	3.48507	1.18747	0.00000
C	–1.96489	–1.30934	0.00000
N	4.86923	1.19815	0.00000
N	–1.85853	1.12754	0.00000
C	5.09608	–1.17405	0.00000
C	–2.51684	–0.03673	0.00000
C	5.63494	0.05779	0.00000
N	–3.87098	–0.24751	0.00000
N	–2.94391	–2.28227	0.00000
C	–4.05829	–1.60892	0.00000
N	0.11184	–2.54102	0.00000
H	–5.04762	–2.04260	0.00000
H	0.07964	1.82739	0.00000
O	3.03447	–2.34040	0.00000
H	–0.40612	–3.40227	0.00000
H	1.13123	–2.54885	0.00000
H	1.90266	–0.12872	0.00000
O	2.82530	2.20365	0.00000
C	5.89628	–2.43872	0.00000
H	6.96697	–2.22451	0.00000
H	5.66023	–3.04521	0.87778
H	5.66023	–3.04521	–0.87778
H	6.70642	0.21987	0.00000
H	–4.57879	0.46780	0.00000
H	5.29536	2.11040	0.00000

Sum of electronic and zero–point Energies: –921.205492 a.u.
N_{Im}= 0

A•T(Hoog)

	X	Y	Z
C	–4.05673	–2.09870	0.00000
C	–2.82160	–2.78007	0.00000

N	–1.50873	–2.35201	0.00000
C	–0.79384	–3.44392	0.00000
N	–1.56429	–4.57275	0.00000
C	–2.87816	–4.16552	0.00000
N	–3.97709	–4.92074	0.00000
C	–5.07352	–4.17019	0.00000
N	–5.17653	–2.83838	0.00000
N	–4.15814	–0.76285	0.00000
O	–2.04312	1.29740	0.00000
C	–0.81992	1.28785	0.00000
N	–0.12863	0.09159	0.00000
C	1.23293	–0.07992	0.00000
O	1.77746	–1.16487	0.00000
N	1.93878	1.10868	0.00000
C	1.33678	2.34482	0.00000
C	0.00116	2.49918	0.00000
C	–0.68889	3.82704	0.00000
H	–5.08269	–0.36756	0.00000
H	–3.35133	–0.14392	0.00000
H	–6.01721	–4.70774	0.00000
H	–1.24402	–5.52672	0.00000
H	0.28695	–3.46182	0.00000
H	–0.69225	–0.78517	0.00000
H	2.94170	1.01963	0.00000
H	2.01598	3.18913	0.00000
H	0.03461	4.64475	0.00000
H	–1.33180	3.92768	0.87780
H	–1.33180	3.92768	–0.87780

Sum of electronic and zero–point Energies: –921.206324 a.u.
N_{Im}= 0

A_{imino}•C

	X	Y	Z
C	–0.57507	1.00515	0.00000
N	–1.86724	1.16516	0.00000
C	–2.51454	–0.02900	0.00000
C	–1.96944	–1.29632	0.00000
C	–0.53874	–1.43532	0.00000
N	0.07224	–0.18277	0.00000
N	–3.86751	–0.22755	0.00000
C	–4.06702	–1.58537	0.00000
N	–2.95013	–2.25907	0.00000
N	0.18990	–2.49698	0.00000
C	3.42771	1.07950	0.00000
N	2.90387	–0.17526	0.00000
C	3.67500	–1.25540	0.00000
C	5.11397	–1.15750	0.00000
C	5.63925	0.08477	0.00000
N	4.83167	1.17393	0.00000
O	2.76142	2.09875	0.00000

N	3.07657	–2.44633	0.00000
H	0.08154	1.86981	0.00000
H	–4.56690	0.49613	0.00000
H	–5.05777	–2.01467	0.00000
H	–0.40685	–3.31877	0.00000
H	5.20819	2.10865	0.00000
H	6.70584	0.27263	0.00000
H	5.74371	–2.03530	0.00000
H	3.63031	–3.28419	0.00000
H	2.03871	–2.51290	0.00000
H	1.11061	–0.16962	0.00000

Sum of electronic and zero–point Energies: –862.007955 a.u.
N_{Im}= 0

A•C$_{imino}$

	X	Y	Z
C	–0.52998	0.91997	0.00000
N	–1.83663	1.13047	0.00000
C	–2.51545	–0.02197	0.00000
C	–1.98684	–1.30415	0.00000
C	–0.58058	–1.40459	0.00000
N	0.11813	–0.25534	0.00000
N	–3.87365	–0.20808	0.00000
C	–4.08588	–1.56581	0.00000
N	–2.98384	–2.25924	0.00000
N	0.06974	–2.57170	0.00000
C	3.45378	1.14289	0.00000
N	2.95278	–0.12948	0.00000
C	3.68071	–1.30977	0.00000
C	5.12769	–1.13756	0.00000
C	5.64490	0.09996	0.00000
N	4.84376	1.21117	0.00000
O	2.76892	2.14283	0.00000
N	3.03527	–2.42043	0.00000
H	0.11546	1.79394	0.00000
H	–4.56806	0.52013	0.00000
H	–5.08301	–1.98128	0.00000
H	–0.46697	–3.42155	0.00000
H	1.09589	–2.59530	0.00000
H	1.91143	–0.19965	0.00000
H	5.23087	2.14026	0.00000
H	6.71118	0.28794	0.00000
H	5.76786	–2.00784	0.00000
H	3.67513	–3.20783	0.00000

Sum of electronic and zero–point Energies: –862.013441 a.u.
N_{Im}= 0

A$_{imino}$•T$_{enol}$

	X	Y	Z
C	–1.48696	–0.07635	0.00000

C	2.66980	–2.53622	0.00000
N	–0.13556	–0.13958	0.00000
N	1.35147	–2.50073	0.00000
C	0.71536	0.95458	0.00000
C	0.59789	–3.64053	0.00000
C	–0.02279	2.18159	0.00000
N	1.30940	–4.84133	0.00000
N	–2.19261	1.01736	0.00000
C	3.41956	–3.77195	0.00000
C	–1.40239	2.12010	0.00000
C	2.67121	–4.89594	0.00000
N	–1.81137	3.42397	0.00000
N	0.41795	3.48293	0.00000
C	–0.67495	4.19414	0.00000
N	1.99402	0.76550	0.00000
H	–0.71965	5.27296	0.00000
H	–1.98101	–1.04241	0.00000
H	2.49171	1.64913	0.00000
H	–2.76709	3.74005	0.00000
H	0.33138	–1.07141	0.00000
H	3.10901	–5.88733	0.00000
C	4.91738	–3.76045	0.00000
H	5.31269	–4.77853	0.00000
H	5.30342	–3.23776	–0.87843
H	5.30342	–3.23776	0.87843
H	0.75425	–5.68234	0.00000
O	–0.62047	–3.64394	0.00000
O	3.35048	–1.43410	0.00000
H	2.75302	–0.56503	0.00000

Sum of electronic and zero–point Energies: –921.184143 a.u.

N_{Im}= 0

A_{imino}•T

	X	Y	Z
N	–0.77724	2.20804	0.00000
C	–0.96377	0.93943	0.00000
N	0.14557	0.08663	0.00000
C	0.08547	–1.26655	0.00000
N	–0.99821	–1.98152	0.00000
C	–2.11136	–1.19929	0.00000
C	–2.18362	0.17720	0.00000
N	–3.48789	0.60546	0.00000
C	–4.19103	–0.49328	0.00000
N	–3.41067	–1.62218	0.00000
C	3.35619	6.92846	0.00000
C	3.19013	5.44188	0.00000
C	1.82191	4.90211	0.00000
O	0.82445	5.59018	0.00000
N	1.72814	3.50805	0.00000
C	2.76731	2.63047	0.00000

O	2.63846	1.40950	0.00000
N	4.01381	3.20826	0.00000
C	4.21186	4.57284	0.00000
H	–5.26936	–0.54700	0.00000
H	1.04833	–1.76614	0.00000
H	–1.66314	2.70369	0.00000
H	–3.71784	–2.58070	0.00000
H	1.06889	0.54122	0.00000
H	0.76571	3.08552	0.00000
H	4.79088	2.56847	0.00000
H	5.24809	4.88896	0.00000
H	4.41205	7.20675	0.00000
H	2.87523	7.36818	–0.87710
H	2.87523	7.36818	0.87710

Sum of electronic and zero–point Energies: –921.189563 a.u.
N_{Im}= 0

I•A

	X	Y	Z
N	–1.30098	–0.22216	0.00000
C	–1.56818	–1.53425	0.00000
C	–0.64675	–2.56893	0.00000
C	0.71702	–2.20707	0.00000
N	1.00611	–0.88913	0.00000
C	0.00069	0.00023	0.00000
H	0.30561	1.04336	0.00000
N	1.69941	–3.10784	0.00000
N	3.75654	–0.00199	0.00000
C	4.73042	–1.01411	0.00000
C	6.04843	–0.44225	0.00000
C	6.17150	0.93808	0.00000
N	5.18868	1.87194	0.00000
C	4.00965	1.32868	0.00000
H	3.13370	1.96914	0.00000
O	4.40593	–2.19177	0.00000
N	7.28467	–1.04409	0.00000
C	8.12897	–0.05366	0.00000
N	7.51507	1.17578	0.00000
N	–2.78881	–2.15541	0.00000
N	–1.27233	–3.79824	0.00000
H	2.68213	–2.82306	0.00000
H	2.76607	–0.31892	0.00000
H	7.95208	2.08255	0.00000
H	9.20474	–0.14925	0.00000
H	1.45646	–4.08370	0.00000
C	–2.54146	–3.50750	0.00000
H	–3.68500	–1.69754	0.00000
H	–3.34569	–4.22857	0.00000

Sum of electronic and zero–point Energies: –954.256253 a.u.
N_{Im}= 0

I•C

	X	Y	Z
N	–3.81306	0.77642	0.00000
C	–4.53850	–0.36887	0.00000
C	–3.92394	–1.56996	0.00000
C	–2.48307	–1.56049	0.00000
N	–1.79263	–0.42848	0.00000
C	–2.40651	0.78583	0.00000
O	–1.81438	1.84920	0.00000
N	–1.79739	–2.70528	0.00000
N	1.03035	–0.23590	0.00000
C	1.68477	–1.47177	0.00000
C	3.10775	–1.28533	0.00000
C	3.60025	0.01158	0.00000
N	2.91245	1.17809	0.00000
C	1.62657	0.97937	0.00000
H	0.94119	1.82119	0.00000
O	1.04522	–2.51822	0.00000
N	4.13570	–2.20035	0.00000
C	5.21636	–1.47558	0.00000
N	4.95861	–0.12570	0.00000
H	–4.25770	1.68087	0.00000
H	–5.61591	–0.25962	0.00000
H	–4.48748	–2.49154	0.00000
H	–2.27794	–3.58674	0.00000
H	–0.76919	–2.68712	0.00000
H	–0.00859	–0.27461	0.00000
H	5.62422	0.62921	0.00000
H	6.22613	–1.85892	0.00000

Sum of electronic and zero–point Energies: –881.906327 a.u.
N_{Im}= 0

I•U

	X	Y	Z
C	–2.67362	–0.04884	0.00000
O	–2.07505	1.02017	0.00000
N	0.72708	1.31627	0.00000
C	1.38711	0.07581	0.00000
C	2.81055	0.26806	0.00000
C	3.30293	1.56379	0.00000
N	2.61116	2.73022	0.00000
C	1.32907	2.53107	0.00000
H	0.65800	3.38329	0.00000
O	0.75161	–0.96689	0.00000
N	3.83700	–0.64606	0.00000
C	4.91806	0.07825	0.00000
N	4.66035	1.42828	0.00000
H	–0.30046	1.26582	0.00000
H	5.32675	2.18271	0.00000

H	5.92760	–0.30547	0.00000
N	–2.06963	–1.26935	0.00000
C	–2.71270	–2.52206	0.00000
C	–4.17269	–2.44268	0.00000
N	–4.05131	–0.07959	0.00000
C	–4.77643	–1.24757	0.00000
H	–1.03655	–1.26337	0.00000
O	–2.07321	–3.54522	0.00000
H	–4.73126	–3.36626	0.00000
H	–4.50414	0.81963	0.00000
H	–5.85227	–1.12785	0.00000

Sum of electronic and zero–point Energies: –901.794287 a.u.
N_{Im}= 0

G•U

	X	Y	Z
C	5.33054	–1.34302	0.00000
O	4.45425	–2.20296	0.00000
N	1.71245	–1.58046	0.00000
C	1.41350	–0.20797	0.00000
C	–0.00088	0.00339	0.00000
C	–0.82680	–1.11197	0.00000
N	–0.49232	–2.42129	0.00000
C	0.80475	–2.59806	0.00000
N	1.31741	–3.85289	0.00000
O	2.32667	0.60667	0.00000
N	–0.74231	1.16566	0.00000
C	–1.97670	0.76499	0.00000
N	–2.09428	–0.61010	0.00000
H	2.71372	–1.80559	0.00000
H	–2.94002	–1.15515	0.00000
H	–2.84563	1.40624	0.00000
N	5.09382	–0.00339	0.00000
C	6.06736	1.01621	0.00000
C	7.44552	0.52689	0.00000
N	6.65933	–1.70402	0.00000
C	7.68676	–0.78960	0.00000
H	4.10043	0.29262	0.00000
O	5.74496	2.17811	0.00000
H	8.24217	1.25515	0.00000
H	6.83941	–2.69445	0.00000
H	8.68433	–1.20973	0.00000
H	0.67720	–4.62551	0.00000
H	2.30859	–4.01574	0.00000

Sum of electronic and zero–point Energies: –957.152734 a.u.
N_{Im}= 1 (220*i* cm^{-1})

A•U

	X	Y	Z
C	–0.54613	0.93960	0.00000

C	3.63657	–1.28353	0.00000
N	0.12211	–0.22526	0.00000
N	2.94582	–0.08235	0.00000
C	–0.55773	–1.38533	0.00000
C	3.48419	1.18094	0.00000
C	–1.96465	–1.30912	0.00000
N	4.87406	1.19865	0.00000
N	–1.85520	1.12757	0.00000
C	5.08618	–1.16001	0.00000
C	–2.51508	–0.03592	0.00000
C	5.63936	0.06391	0.00000
N	–3.86952	–0.24494	0.00000
N	–2.94476	–2.28079	0.00000
C	–4.05835	–1.60620	0.00000
N	0.10978	–2.54395	0.00000
H	–5.04818	–2.03872	0.00000
H	0.08341	1.82508	0.00000
O	3.03420	–2.34758	0.00000
H	–0.40979	–3.40427	0.00000
H	1.12900	–2.55454	0.00000
H	1.90084	–0.13282	0.00000
O	2.82826	2.19814	0.00000
H	6.71056	0.22223	0.00000
H	–4.57653	0.47116	0.00000
H	5.29401	2.11400	0.00000
H	5.68214	–2.05957	0.00000

Sum of electronic and zero–point Energies: –881.915538 a.u.

N_{Im}= 0

C•C

	X	Y	Z
C	–0.63625	2.04287	0.00000
N	–1.56860	1.09079	0.00000
N	–0.63634	–1.66475	0.00000
C	0.63625	–2.04287	0.00000
C	1.02070	–3.43371	0.00000
C	0.02253	–4.34004	0.00000
N	–1.27102	–3.93497	0.00000
C	–1.64660	–2.57600	0.00000
O	–2.82999	–2.29191	0.00000
N	1.56860	–1.09079	0.00000
N	0.63633	1.66475	0.00000
C	1.64660	2.57600	0.00000
N	1.27101	3.93497	0.00000
C	–1.02070	3.43371	0.00000
C	–0.02253	4.34004	0.00000
O	2.82999	2.29191	0.00000
H	2.03033	4.59714	0.00000
H	–2.05792	3.73578	0.00000
H	–0.19676	5.40906	0.00000

H	–2.54514	1.32454	0.00000
H	–1.28988	0.09837	0.00000
H	2.54514	–1.32454	0.00000
H	1.28987	–0.09837	0.00000
H	–2.03033	–4.59714	0.00000
H	2.05792	–3.73578	0.00000
H	0.19675	–5.40906	0.00000

Sum of electronic and zero–point Energies: –789.664831 a.u.
N_{Im}= 0

G•G

	X	Y	Z
C	1.98793	–0.48250	0.00000
O	1.68661	0.71369	0.00000
N	–0.97783	1.44589	0.00000
C	–1.98792	0.48251	0.00000
C	–3.27848	1.08545	0.00000
C	–3.34606	2.47384	0.00000
N	–2.34300	3.37405	0.00000
C	–1.16385	2.79843	0.00000
N	–0.03675	3.54309	0.00000
O	–1.68660	–0.71368	0.00000
N	–4.54096	0.52908	0.00000
C	–5.34457	1.54793	0.00000
N	–4.67958	2.75756	0.00000
H	–0.00005	1.10671	0.00000
H	–5.08148	3.68010	0.00000
H	–6.42332	1.49703	0.00000
N	0.97784	–1.44589	0.00000
C	1.16386	–2.79842	0.00000
N	2.34301	–3.37405	0.00000
C	3.27849	–1.08545	0.00000
C	3.34607	–2.47383	0.00000
H	0.00006	–1.10670	0.00000
N	0.03676	–3.54309	0.00000
N	4.54098	–0.52907	0.00000
N	4.67960	–2.75755	0.00000
H	–0.12710	4.54244	0.00000
H	0.87426	3.11323	0.00000
H	0.12712	–4.54244	0.00000
H	–0.87424	–3.11322	0.00000
C	5.34458	–1.54793	0.00000
H	6.42333	–1.49702	0.00000
H	5.08150	–3.68009	0.00000

Sum of electronic and zero–point Energies: –1084.864616 a.u.
N_{Im}= 1 (7*i* cm^{-1})

8-oxoG•A

	X	Y	Z
C	–2.67185	1.63132	0.00000

C	–2.75364	0.22719	0.00000
N	–1.77456	–0.75452	0.00000
C	–2.35874	–1.99245	0.00000
N	–3.74643	–1.73603	0.00000
C	–3.98427	–0.39259	0.00000
N	–5.19581	0.19807	0.00000
C	–5.13978	1.50467	0.00000
N	–3.96693	2.20338	0.00000
N	1.18292	1.85876	0.00000
C	1.77561	0.66019	0.00000
N	1.03291	–0.45957	0.00000
C	3.17678	0.50499	0.00000
N	–6.29376	2.21908	0.00000
O	–1.83606	–3.08558	0.00000
H	–0.74779	–0.60146	0.00000
C	1.63610	–1.66021	0.00000
C	3.65582	–0.79632	0.00000
H	–3.96852	3.21338	0.00000
H	–6.31546	3.22129	0.00000
H	–7.15686	1.70585	0.00000
H	1.76173	2.68067	0.00000
N	2.93254	–1.92121	0.00000
H	0.95974	–2.51152	0.00000
N	4.20944	1.42090	0.00000
N	5.02006	–0.66288	0.00000
C	5.28412	0.68557	0.00000
H	6.29636	1.06269	0.00000
H	0.16871	1.95845	0.00000
O	–1.68938	2.36846	0.00000
H	5.68586	–1.41741	0.00000
H	–4.43968	–2.46463	0.00000

Sum of electronic and zero–point Energies: –1084.862524 a.u.
N_{Im}= 1 (329*i* cm^{-1})

Reverse A•U

	X	Y	Z
C	–0.54693	0.92910	0.00000
C	3.60887	–1.24171	0.00000
N	0.12241	–0.23552	0.00000
N	2.94279	–0.05229	0.00000
C	–0.55544	–1.39562	0.00000
C	3.50549	1.22688	0.00000
C	–1.96199	–1.32262	0.00000
C	4.96583	1.24003	0.00000
N	–1.85647	1.11418	0.00000
N	4.98685	–1.12949	0.00000
C	–2.51439	–0.05004	0.00000
C	5.63789	0.07955	0.00000
N	–3.86851	–0.26138	0.00000
N	–2.94057	–2.29591	0.00000

C	–4.05513	–1.62287	0.00000
N	0.11392	–2.55460	0.00000
H	–5.04430	–2.05692	0.00000
H	0.08252	1.81475	0.00000
O	3.06057	–2.33234	0.00000
H	–0.40421	–3.41571	0.00000
H	1.13152	–2.56411	0.00000
H	1.89872	–0.11200	0.00000
O	2.79681	2.21104	0.00000
H	6.71923	0.02584	0.00000
H	–4.57667	0.45362	0.00000
H	5.47139	2.19364	0.00000
H	5.49438	–1.99910	0.00000

Sum of electronic and zero–point Energies: –881.914785 a.u.
N_{Im}= 0

Reverse A•U(Hoog)

	X	Y	Z
C	–4.06659	–2.08823	0.00000
C	–2.83248	–2.77028	0.00000
N	–1.51924	–2.34373	0.00000
C	–0.80526	–3.43641	0.00000
N	–1.57699	–4.56413	0.00000
C	–2.89041	–4.15579	0.00000
N	–3.99042	–4.90925	0.00000
C	–5.08599	–4.15774	0.00000
N	–5.18728	–2.82553	0.00000
N	–4.16685	–0.75126	0.00000
O	–2.01986	1.31728	0.00000
C	–0.80272	1.24800	0.00000
N	–0.10649	0.07559	0.00000
C	1.27931	–0.08354	0.00000
O	1.77060	–1.19487	0.00000
C	2.02640	1.16975	0.00000
C	1.36062	2.33482	0.00000
N	–0.01119	2.38232	0.00000
H	–5.09062	–0.35434	0.00000
H	–3.35983	–0.13509	0.00000
H	–6.03031	–4.69410	0.00000
H	–1.25724	–5.51831	0.00000
H	0.27569	–3.45388	0.00000
H	–0.67697	–0.79741	0.00000
H	3.10489	1.12801	0.00000
H	1.85929	3.29582	0.00000
H	–0.50567	3.25955	0.00000

Sum of electronic and zero–point Energies: –881.915814 a.u.
N_{Im}= 0

Reverse G•U

	X	Y	Z

C	–0.00710	0.06116	0.00000
O	0.96152	0.81846	0.00000
N	3.62121	–0.01900	0.00000
C	3.82531	–1.40684	0.00000
C	5.22124	–1.71618	0.00000
C	6.12183	–0.65982	0.00000
N	5.87853	0.66903	0.00000
C	4.59586	0.93419	0.00000
N	4.16825	2.21982	0.00000
O	2.85720	–2.15746	0.00000
N	5.88134	–2.92673	0.00000
C	7.14028	–2.61157	0.00000
N	7.35193	–1.24779	0.00000
H	2.63610	0.27684	0.00000
H	8.23304	–0.76203	0.00000
H	7.96323	–3.31087	0.00000
N	0.16312	–1.31019	0.00000
C	–0.84069	–2.26166	0.00000
N	–2.12387	–1.71747	0.00000
C	–1.38091	0.52500	0.00000
C	–2.37705	–0.37727	0.00000
H	1.13420	–1.67727	0.00000
O	–0.65324	–3.45040	0.00000
H	–2.87146	–2.39275	0.00000
H	–1.56662	1.58768	0.00000
H	–3.42256	–0.09534	0.00000
H	4.85797	2.94852	0.00000
H	3.18933	2.44717	0.00000

Sum of electronic and zero–point Energies: –957.155034 a.u.
N_{Im}= 1 (192*i* cm^{-1})

A•yT

	X	Y	Z
C	–0.66660	–1.13550	0.00000
C	3.44115	1.14518	0.00000
N	–0.02670	0.04527	0.00000
N	2.79827	–0.06470	0.00000
C	–0.73371	1.18812	0.00000
C	3.38432	–1.32005	0.00000
C	–2.13819	1.07930	0.00000
C	4.86119	–1.31270	0.00000
N	–1.97093	–1.35412	0.00000
N	4.81204	1.08467	0.00000
C	–2.65821	–0.20685	0.00000
C	5.54380	–0.09411	0.00000
N	–4.01713	–0.02992	0.00000
N	–3.14116	2.02748	0.00000
C	–4.23834	1.32636	0.00000
N	–0.09347	2.36295	0.00000
H	–5.23821	1.73518	0.00000

H	–0.01528	–2.00512	0.00000
O	2.84849	2.21299	0.00000
H	–0.63259	3.21108	0.00000
H	0.92399	2.39661	0.00000
H	1.75338	–0.02702	0.00000
O	2.70675	–2.32545	0.00000
C	6.94030	–0.07610	0.00000
H	–4.70695	–0.76263	0.00000
H	5.28116	1.97648	0.00000
H	7.47051	0.87007	0.00000
C	7.63458	–1.27269	0.00000
H	8.71856	–1.25497	0.00000
C	6.95950	–2.49533	0.00000
H	7.51636	–3.42413	0.00000
C	5.57737	–2.50937	0.00000
H	5.01679	–3.43670	0.00000

Sum of electronic and zero–point Energies: –1035.504182 a.u.
N_{Im}= 0

G•yC

	X	Y	Z
C	0.06143	1.18891	0.00000
N	0.03253	–0.12864	0.00000
C	1.18787	–0.86085	0.00000
O	1.15663	–2.08760	0.00000
C	2.47731	–0.13172	0.00000
C	2.46304	1.26215	0.00000
N	1.22809	1.89874	0.00000
N	–1.08613	1.86779	0.00000
C	–3.60848	–0.74665	0.00000
C	–4.82183	–1.49585	0.00000
C	–4.72741	–2.88137	0.00000
N	–3.62903	–3.65850	0.00000
C	–2.51557	–2.95521	0.00000
N	–2.49017	–1.58531	0.00000
O	–3.45860	0.47516	0.00000
N	–1.32305	–3.57535	0.00000
N	–6.14130	–1.08942	0.00000
C	–6.82141	–2.19443	0.00000
N	–6.02007	–3.31881	0.00000
C	3.65528	1.98754	0.00000
H	1.20026	2.90526	0.00000
H	–1.33227	–4.57912	0.00000
H	–0.43724	–3.06737	0.00000
H	–7.89885	–2.26920	0.00000
H	–1.98240	1.34680	0.00000
H	–1.10358	2.87188	0.00000
H	–1.57689	–1.10414	0.00000
H	–6.31081	–4.28190	0.00000
H	3.63633	3.07235	0.00000

C	4.85748	1.30324	0.00000
H	5.78591	1.86280	0.00000
C	4.88658	–0.09351	0.00000
H	5.83567	–0.61541	0.00000
C	3.70024	–0.80325	0.00000
H	3.68361	–1.88651	0.00000

Sum of electronic and zero–point Energies: –1090.849309 a.u.
N_{Im}= 1 (18*i* cm^{-1})

IsoC•IsoG

	X	Y	Z
C	0.052180	1.237450	0.000000
N	0.046500	–0.137540	0.000000
C	1.164960	–0.826370	0.000000
N	1.128960	–2.158590	0.000000
N	2.389280	–0.203900	0.000000
C	2.466770	1.171040	0.000000
C	1.351470	1.912050	0.000000
C	–3.637140	–0.741960	0.000000
C	–4.816210	–1.488410	0.000000
C	–4.673500	–2.877990	0.000000
N	–3.571160	–3.613710	0.000000
C	–2.433140	–2.897770	0.000000
N	–2.505810	–1.481220	0.000000
N	–3.566610	0.587350	0.000000
O	–1.296400	–3.389530	0.000000
N	–6.146150	–1.107100	0.000000
C	–6.794200	–2.231020	0.000000
N	–5.965610	–3.336030	0.000000
H	–7.869560	–2.331970	0.000000
H	–6.235880	–4.305220	0.000000
H	–2.668460	1.083180	0.000000
H	–4.430440	1.102050	0.000000
O	–1.003660	1.867430	0.000000
H	3.232960	–0.751880	0.000000
H	3.467120	1.584050	0.000000
H	–1.595560	–0.994310	0.000000
H	1.384330	2.991570	0.000000
H	1.970180	–2.707060	0.000000
H	0.203410	–2.639530	0.000000

Sum of electronic and zero–point Energies: –937.256417 a.u.
N_{Im}= 0

K•Pi

	X	Y	Z
C	0.14595	1.22543	0.00000
N	0.07169	–0.12203	0.00000
C	1.23426	–0.79231	0.00000
N	1.18223	–2.13988	0.00000
C	2.46715	–0.10930	0.00000

C	2.40377	1.26408	0.00000
N	1.26701	1.95895	0.00000
C	–3.64703	–0.71767	0.00000
C	–4.85875	–1.50508	0.00000
C	–4.84348	–2.88275	0.00000
N	–3.64215	–3.56039	0.00000
C	–2.44087	–2.89537	0.00000
N	–2.50923	–1.51118	0.00000
O	–3.59262	0.49995	0.00000
O	–1.38055	–3.49519	0.00000
N	–6.16404	–1.12815	0.00000
N	–6.96658	–2.18224	0.00000
C	–6.19133	–3.26688	0.00000
N	–1.01632	1.90949	0.00000
H	–1.58793	–1.01716	0.00000
H	2.03445	–2.66870	0.00000
H	0.29554	–2.63497	0.00000
H	–0.95870	2.91148	0.00000
H	–1.91605	1.44511	0.00000
H	–3.58942	–4.56581	0.00000
C	–6.70144	0.22056	0.00000
H	–7.78510	0.12791	0.00000
H	–6.36529	0.75680	0.88728
H	–6.36529	0.75680	–0.88728
H	3.31765	1.85305	0.00000
H	3.40930	–0.64080	0.00000
H	–6.63218	–4.25100	0.00000

Sum of electronic and zero–point Energies: –976.532423 a.u.
N_{Im}= 2 (134*i* cm^{-1}, 20*i* cm^{-1})

T(h)•G

	X	Y	Z
C	0.08680	1.03351	0.00000
N	0.15292	–0.26801	0.00000
C	1.36385	–0.91865	0.00000
N	2.48584	–0.09451	0.00000
C	2.42134	1.26298	0.00000
C	1.22004	1.89750	0.00000
C	–3.42707	–0.69092	0.00000
C	–4.67854	–1.39280	0.00000
C	–4.64879	–2.78065	0.00000
N	–3.58821	–3.61727	0.00000
C	–2.44745	–2.96579	0.00000
N	–2.35699	–1.60573	0.00000
O	–3.19236	0.50679	0.00000
N	–1.27698	–3.64364	0.00000
N	–5.97749	–0.92803	0.00000
C	–6.70944	–2.00041	0.00000
N	–5.96060	–3.15892	0.00000
H	–7.78918	–2.02507	0.00000

H	–6.29428	–4.10786	0.00000
H	3.37786	–0.56745	0.00000
H	3.37068	1.78590	0.00000
H	–1.42505	–1.17084	0.00000
C	1.06650	3.39066	0.00000
H	2.03859	3.88740	0.00000
H	0.51496	3.72693	–0.88144
H	0.51496	3.72693	0.88144
O	1.47586	–2.13137	0.00000
H	–0.92716	1.43956	0.00000
H	–0.37505	–3.18121	0.00000
H	–1.32471	–4.64601	0.00000

Sum of electronic and zero–point Energies: –921.181735 a.u.
N_{Im}= 1 (16*i* cm^{-1})

K•X

	X	Y	Z
C	–3.97597	0.80638	0.00000
C	–4.54026	–0.44802	0.00000
N	–3.84109	–1.58109	0.00000
C	–2.50812	–1.43489	0.00000
N	–1.83346	–0.26511	0.00000
C	–2.56792	0.85682	0.00000
N	–1.78130	–2.56866	0.00000
N	1.10548	–0.19586	0.00000
C	1.76612	–1.43857	0.00000
C	3.20733	–1.29739	0.00000
C	3.76287	–0.04568	0.00000
N	3.04106	1.11418	0.00000
C	1.65437	1.06074	0.00000
O	1.00132	2.08834	0.00000
O	1.13672	–2.47385	0.00000
N	4.19630	–2.25609	0.00000
C	5.30889	–1.59388	0.00000
N	5.10869	–0.22024	0.00000
H	–2.28456	–3.43708	0.00000
H	–0.76774	–2.56162	0.00000
H	0.06152	–0.22539	0.00000
H	5.82145	0.49010	0.00000
H	6.30293	–2.01433	0.00000
H	3.44884	2.03490	0.00000
N	–1.91200	2.03679	0.00000
H	–0.89823	2.07706	0.00000
H	–2.43305	2.89365	0.00000
H	–4.57599	1.70648	0.00000
H	–5.62182	–0.56010	0.00000

Sum of electronic and zero–point Energies: –937.263729 a.u.
N_{Im}= 1 (23*i* cm^{-1})

G•C

	X	Y	Z
C	0.00616	1.32505	0.00000
N	–0.00322	–0.00585	0.00000
C	1.15113	–0.71341	0.00000
O	1.20614	–1.93763	0.00000
N	2.35014	0.00979	0.00000
C	2.38379	1.36619	0.00000
C	1.23751	2.07505	0.00000
N	–1.16480	1.95601	0.00000
C	–3.62733	–0.75111	0.00000
C	–4.81379	–1.54393	0.00000
C	–4.67088	–2.92493	0.00000
N	–3.54552	–3.66349	0.00000
C	–2.45777	–2.92185	0.00000
N	–2.47958	–1.55243	0.00000
O	–3.51866	0.47335	0.00000
N	–1.24482	–3.50348	0.00000
N	–6.14655	–1.18423	0.00000
C	–6.78765	–2.31236	0.00000
N	–5.94733	–3.40782	0.00000
H	3.36365	1.82675	0.00000
H	1.24332	3.15530	0.00000
H	–1.22251	–4.50703	0.00000
H	–0.37514	–2.97110	0.00000
H	–7.86181	–2.42481	0.00000
H	–2.04804	1.41928	0.00000
H	–1.19769	2.95982	0.00000
H	–1.58507	–1.03863	0.00000
H	3.19522	–0.53934	0.00000
H	–6.20397	–4.38053	0.00000

Sum of electronic and zero–point Energies: –937.271742 a.u.
N_{Im}= 0

Reverse G•C

	X	Y	Z
C	–1.03272	–0.84626	0.00000
C	2.89211	0.91383	0.00000
N	–0.97616	0.51685	0.00000
N	3.10552	–0.43231	0.00000
C	–2.08899	1.39983	0.00000
C	4.33415	–0.90913	0.00000
C	–3.31550	0.64638	0.00000
C	5.50267	–0.07455	0.00000
N	–2.15132	–1.53384	0.00000
N	4.02448	1.74243	0.00000
C	–3.24215	–0.73573	0.00000
C	5.28697	1.25902	0.00000
N	–4.54049	–1.15917	0.00000
N	–4.62841	1.06947	0.00000
C	–5.32659	–0.02555	0.00000

H	–6.40500	–0.08464	0.00000
N	0.14607	–1.51314	0.00000
O	1.79077	1.43233	0.00000
N	4.48049	–2.24864	0.00000
H	6.08789	1.98752	0.00000
H	–4.84304	–2.11829	0.00000
H	6.50167	–0.48499	0.00000
H	3.83669	2.73377	0.00000
H	0.08801	–2.51485	0.00000
H	1.05084	–1.05933	0.00000
H	–0.05925	0.96470	0.00000
O	–1.91147	2.59783	0.00000
H	5.38547	–2.68190	0.00000
H	3.65740	–2.82626	0.00000

Sum of electronic and zero–point Energies: –937.249539 a.u.
N_{Im}= 2 (74*i* cm^{-1}, 4*i* cm^{-1})

Reverse A•C

	X	Y	Z
C	2.73612	–0.52893	0.00000
N	–0.99005	–1.18012	0.00000
C	–1.52144	0.06125	0.00000
C	–2.93055	0.15996	0.00000
C	–3.64023	–1.02991	0.00000
N	–3.13209	–2.26866	0.00000
C	–1.80976	–2.24016	0.00000
N	–3.77792	1.24920	0.00000
C	–4.96927	0.72448	0.00000
N	–4.95689	–0.65016	0.00000
H	–5.75000	–1.26930	0.00000
N	2.17638	0.66968	0.00000
C	2.93286	1.80394	0.00000
N	4.33296	1.62524	0.00000
C	4.16587	–0.71339	0.00000
C	4.92006	0.40522	0.00000
O	2.48373	2.93221	0.00000
H	4.87883	2.47231	0.00000
H	4.61422	–1.69631	0.00000
H	6.00301	0.38635	0.00000
H	–5.89517	1.28084	0.00000
N	–0.72331	1.12620	0.00000
H	–1.13382	2.04430	0.00000
H	0.29752	1.02280	0.00000
H	–1.31360	–3.20735	0.00000
N	1.92653	–1.59466	0.00000
H	2.31326	–2.52095	0.00000
H	0.90420	–1.46453	0.00000

Sum of electronic and zero–point Energies: –862.016609 a.u.
N_{Im}= 0

P•Z

	X	Y	Z
C	2.44094	–1.41493	0.00000
N	1.90420	–0.12956	0.00000
C	2.59953	1.04014	0.00000
C	4.00696	0.93750	0.00000
C	4.60736	–0.34385	0.00000
C	3.87538	–1.48475	0.00000
O	1.67828	–2.38101	0.00000
N	1.89631	2.16750	0.00000
H	4.32868	–2.46544	0.00000
H	5.68952	–0.37708	0.00000
N	4.84748	2.08499	0.00000
H	2.42159	3.02961	0.00000
H	0.87423	2.16521	0.00000
N	–1.01204	–0.10197	0.00000
C	–1.57388	1.11397	0.00000
N	–2.99356	1.11697	0.00000
C	–3.67309	–0.06183	0.00000
N	–3.13263	–1.25051	0.00000
C	–1.77425	–1.21433	0.00000
N	–1.14157	–2.38217	0.00000
O	–0.98799	2.18569	0.00000
C	–3.88802	2.18506	0.00000
C	–5.12176	1.65012	0.00000
N	–4.98547	0.26263	0.00000
H	–0.11559	–2.42086	0.00000
H	–1.69335	–3.22187	0.00000
H	–5.72302	–0.42101	0.00000
H	–6.08723	2.12445	0.00000
H	–3.54058	3.20270	0.00000
H	0.87041	–0.09150	0.00000
O	6.05760	1.92270	0.00000
O	4.32776	3.20577	0.00000

Sum of electronic and zero–point Energies: –1125.708363 a.u.
N_{Im}= 0

G•A_{imino}

	X	Y	Z
C	–2.60005	1.05099	0.00000
C	–2.88838	–0.34686	0.00000
N	–2.04012	–1.43220	0.00000
C	–2.83085	–2.46354	0.00000
N	–4.16339	–2.11241	0.00000
C	–4.21259	–0.75039	0.00000
N	–5.32889	0.01074	0.00000
C	–5.06808	1.29055	0.00000
N	–3.79623	1.80346	0.00000
N	1.87464	2.67259	0.00000
C	2.11962	1.42197	0.00000

N	1.12656	0.40858	0.00000
C	3.43053	0.80483	0.00000
N	–6.08956	2.17948	0.00000
C	1.35165	–0.92943	0.00000
C	3.52199	–0.57151	0.00000
H	–3.64956	2.80333	0.00000
H	–5.94971	3.17249	0.00000
H	–7.02495	1.81361	0.00000
N	2.51802	–1.49665	0.00000
H	0.44961	–1.53295	0.00000
N	4.68041	1.37540	0.00000
N	4.86141	–0.84518	0.00000
C	5.50563	0.36628	0.00000
H	6.58322	0.43786	0.00000
H	0.87123	2.84653	0.00000
O	–1.52931	1.63140	0.00000
H	5.27201	–1.76339	0.00000
H	–4.95869	–2.72969	0.00000
H	0.15616	0.72238	0.00000
H	–2.51643	–3.49639	0.00000

Sum of electronic and zero–point Energies: –1009.576579 a.u.
N_{Im}= 1 (282*i* cm^{-1})

Syn-G•A

	X	Y	Z
C	–2.76630	1.65675	0.00000
C	–2.83672	0.24046	0.00000
N	–1.88567	–0.77286	0.00000
C	–2.58630	–1.87521	0.00000
N	–3.93243	–1.65948	0.00000
C	–4.11705	–0.29898	0.00000
N	–5.27707	0.35564	0.00000
C	–5.07988	1.66978	0.00000
N	–3.92735	2.33667	0.00000
O	1.09327	1.66645	0.00000
C	1.77043	0.65090	0.00000
N	1.14084	–0.60854	0.00000
C	3.19436	0.51343	0.00000
C	1.78668	–1.81152	0.00000
C	3.73004	–0.76421	0.00000
N	3.08668	–1.95233	0.00000
N	0.99980	–2.91667	0.00000
N	4.19095	1.46595	0.00000
N	5.08067	–0.58102	0.00000
C	5.29451	0.78232	0.00000
H	6.29129	1.19778	0.00000
N	–1.63008	2.35321	0.00000
H	5.77237	–1.31180	0.00000
H	–4.66424	–2.35044	0.00000
H	1.44566	–3.81560	0.00000

H	0.00118	–2.84422	0.00000
H	0.11230	–0.59471	0.00000
H	–1.71218	3.35621	0.00000
H	–0.69619	1.94196	0.00000
H	–5.97451	2.28568	0.00000
H	–2.18793	–2.87981	0.00000

Sum of electronic and zero–point Energies: –1009.609454 a.u.
N_{Im}= 2 (391*i* cm^{-1}, 33*i* cm^{-1})

G•A

	X	Y	Z
N	–4.20153	0.81005	0.00000
C	–4.40813	–0.51324	0.00000
C	–3.43737	–1.49981	0.00000
C	–2.09052	–1.07509	0.00000
N	–1.85941	0.25687	0.00000
C	–2.91161	1.08974	0.00000
H	–2.67283	2.15110	0.00000
N	–1.07752	–1.93824	0.00000
N	1.00365	1.12704	0.00000
C	1.96463	0.09883	0.00000
C	3.29067	0.63399	0.00000
C	3.44102	2.01177	0.00000
N	2.48800	2.96831	0.00000
C	1.28008	2.46403	0.00000
N	0.21267	3.29958	0.00000
O	1.60533	–1.06994	0.00000
N	4.51720	0.00395	0.00000
C	5.38079	0.97297	0.00000
N	4.78841	2.21948	0.00000
N	–5.59707	–1.19264	0.00000
N	–4.00124	–2.75836	0.00000
H	–0.09949	–1.63065	0.00000
H	0.01754	0.82179	0.00000
H	5.24364	3.11679	0.00000
H	6.45457	0.85792	0.00000
H	–1.29093	–2.92138	0.00000
C	–5.28327	–2.53105	0.00000
H	–6.51484	–0.77975	0.00000
H	–6.05086	–3.29098	0.00000
H	0.38602	4.28798	0.00000
H	–0.72773	2.95268	0.00000

Sum of electronic and zero–point Energies: –1009.612758 a.u.
N_{Im}= 2 (332*i* cm^{-1}, 26*i* cm^{-1})

U•U 1

	X	Y	Z
C	–1.77146	1.36836	0.00000
C	1.68049	–0.79495	0.00000
O	–1.76493	0.14777	0.00000

O	1.62814	0.42548	0.00000
N	–0.64842	2.14453	0.00000
N	0.51922	–1.55583	0.00000
C	–0.59625	3.54864	0.00000
C	0.42974	–2.93198	0.00000
C	–1.90823	4.19237	0.00000
N	1.66704	–3.56727	0.00000
N	–2.95922	2.07106	0.00000
C	2.91748	–1.55782	0.00000
C	–3.01916	3.44319	0.00000
C	2.86084	–2.89935	0.00000
H	0.24325	1.63083	0.00000
H	–0.36821	–1.03636	0.00000
O	0.46394	4.12833	0.00000
O	–0.60795	–3.54755	0.00000
H	–1.94567	5.27103	0.00000
H	1.63035	–4.57372	0.00000
H	–3.79373	1.50742	0.00000
H	3.85282	–1.02002	0.00000
H	–4.01583	3.86579	0.00000
H	3.74616	–3.52279	0.00000

Sum of electronic and zero–point Energies: –829.451450 a.u.
N_{Im}= 0

U•U 2

	X	Y	Z
C	–1.77458	1.38708	0.00000
C	1.61458	–0.81708	0.00000
O	–1.77463	0.16740	0.00000
O	1.61463	0.40260	0.00000
N	–0.64628	2.15712	0.00000
N	0.48628	–1.58712	0.00000
C	–0.58344	3.56035	0.00000
C	0.42344	–2.99035	0.00000
C	–1.89037	4.21330	0.00000
C	1.73037	–3.64330	0.00000
N	–2.95697	2.09913	0.00000
N	2.79697	–1.52913	0.00000
C	–3.00654	3.47149	0.00000
C	2.84654	–2.90149	0.00000
H	0.24083	1.63910	0.00000
H	–0.40083	–1.06910	0.00000
O	0.48205	4.13105	0.00000
O	–0.64205	–3.56105	0.00000
H	–1.92061	5.29217	0.00000
H	1.76061	–4.72217	0.00000
H	–3.79588	1.54189	0.00000
H	3.63588	–0.97189	0.00000
H	–4.00007	3.90140	0.00000
H	3.84007	–3.33140	0.00000

Sum of electronic and zero–point Energies: –829.450726 a.u.
N_{Im}= 0

U•U 3

	X	Y	Z
C	–3.58329	–1.21161	0.00000
C	2.54329	0.94161	0.00000
O	–3.63733	–2.41651	0.00000
O	2.59733	2.14651	0.00000
N	–2.41228	–0.48272	0.00000
N	1.37228	0.21272	0.00000
C	–2.29229	0.89944	0.00000
C	1.25229	–1.16944	0.00000
C	–3.54841	1.62995	0.00000
C	2.50841	–1.89995	0.00000
N	–4.72834	–0.42078	0.00000
N	3.68834	0.15078	0.00000
C	–4.70422	0.94640	0.00000
C	3.66422	–1.21640	0.00000
H	–1.53290	–1.01938	0.00000
H	0.49290	0.74938	0.00000
O	–1.19210	1.43240	0.00000
O	0.15210	–1.70240	0.00000
H	–3.51585	2.70836	0.00000
H	2.47585	–2.97836	0.00000
H	–5.59771	–0.92920	0.00000
H	4.55771	0.65920	0.00000
H	–5.67200	1.43216	0.00000
H	4.63200	–1.70216	0.00000

Sum of electronic and zero–point Energies: –829.452237 a.u.
N_{Im}= 0

A•4-thioU

	X	Y	Z
C	–1.42626	–1.02455	0.00000
C	3.16117	0.38613	0.00000
N	–0.67004	0.08859	0.00000
N	2.14899	–0.53921	0.00000
C	–1.27075	1.29130	0.00000
C	2.29568	–1.91263	0.00000
C	–2.67867	1.31929	0.00000
N	3.61272	–2.34300	0.00000
N	–2.74627	–1.11530	0.00000
C	4.49829	–0.15521	0.00000
C	–3.32140	0.09125	0.00000
C	4.67884	–1.48775	0.00000
N	–4.65688	0.39959	0.00000
N	–3.58382	2.36157	0.00000
C	–4.74432	1.77126	0.00000

N	–0.52996	2.40496	0.00000
H	–5.69932	2.27606	0.00000
H	–0.86448	–1.95312	0.00000
S	2.87024	2.02362	0.00000
H	–0.98777	3.29969	0.00000
H	0.48467	2.34265	0.00000
H	1.15577	–0.21583	0.00000
O	1.36856	–2.68912	0.00000
H	5.65772	–1.94984	0.00000
H	–5.41505	–0.26208	0.00000
H	3.73831	–3.34262	0.00000
H	5.33378	0.52697	0.00000

Sum of electronic and zero–point Energies: –1204.874211 a.u.
N_{Im}= 0

G•4-thioU

	X	Y	Z
C	2.46831	–0.09963	0.00000
O	1.58790	–0.95321	0.00000
N	–1.16611	–0.37308	0.00000
C	–1.45706	1.00131	0.00000
C	–2.86987	1.22146	0.00000
C	–3.70254	0.11118	0.00000
N	–3.37569	–1.20017	0.00000
C	–2.08001	–1.38520	0.00000
N	–1.57637	–2.64387	0.00000
O	–0.53906	1.81033	0.00000
N	–3.60421	2.38810	0.00000
C	–4.84097	1.99490	0.00000
N	–4.96696	0.62050	0.00000
H	–0.16578	–0.59893	0.00000
H	–5.81601	0.08059	0.00000
H	–5.70597	2.64144	0.00000
N	2.22980	1.24485	0.00000
C	3.19028	2.24925	0.00000
C	4.55835	1.77437	0.00000
N	3.79438	–0.46039	0.00000
C	4.81712	0.45859	0.00000
H	1.23094	1.52519	0.00000
S	2.77501	3.83999	0.00000
H	5.35361	2.50348	0.00000
H	3.97596	–1.45075	0.00000
H	5.81876	0.04931	0.00000
H	–2.22255	–3.41156	0.00000
H	–0.58685	–2.81517	0.00000

Sum of electronic and zero–point Energies: –1280.112362 a.u.
N_{Im}= 1 (225*i* cm^{-1})

G•2-thioU

	X	Y	Z

C	2.78186	–0.21863	0.00000
S	1.86412	–1.62684	0.00000
N	–1.31511	–0.58339	0.00000
C	–1.45312	0.81485	0.00000
C	–2.83211	1.19019	0.00000
C	–3.78250	0.17917	0.00000
N	–3.60215	–1.15969	0.00000
C	–2.33595	–1.48962	0.00000
N	–1.98258	–2.79769	0.00000
O	–0.45268	1.51844	0.00000
N	–3.43240	2.43112	0.00000
C	–4.70503	2.17719	0.00000
N	–4.98258	0.82511	0.00000
H	–0.34494	–0.91276	0.00000
H	–5.88627	0.38261	0.00000
H	–5.49309	2.91556	0.00000
N	2.29692	1.03799	0.00000
C	3.06344	2.23082	0.00000
C	4.50620	2.01174	0.00000
N	4.14361	–0.32185	0.00000
C	4.98707	0.76236	0.00000
H	1.26696	1.17207	0.00000
O	2.52236	3.30625	0.00000
H	5.15227	2.87652	0.00000
H	4.50862	–1.26108	0.00000
H	6.04395	0.52892	0.00000
H	–2.71585	–3.48291	0.00000
H	–1.02261	–3.09063	0.00000

Sum of electronic and zero–point Energies: –1280.107407 a.u.
N_{Im}= 2 (253*i* cm^{-1}, 8*i* cm^{-1})

G•G 3

	X	Y	Z
N	–2.21946	–3.65198	0.00000
C	–1.29261	–2.58290	0.00000
C	–1.98437	–1.33748	0.00000
C	–3.36525	–1.32396	0.00000
N	–4.21075	–2.37902	0.00000
C	–3.58724	–3.52636	0.00000
N	–4.30738	–4.67472	0.00000
O	–0.09584	–2.80803	0.00000
N	–1.48692	–0.05902	0.00000
C	–2.52966	0.71942	0.00000
N	–3.70248	–0.00024	0.00000
H	–1.79383	–4.56821	0.00000
H	–3.88596	–5.58445	0.00000
H	–5.30860	–4.59514	0.00000
H	–4.63872	0.36996	0.00000
H	–2.47915	1.79992	0.00000
N	1.03214	1.25227	0.00000

C	0.81964	2.64560	0.00000
C	2.07564	3.34014	0.00000
C	3.23956	2.58500	0.00000
N	3.39169	1.24349	0.00000
C	2.23675	0.61517	0.00000
N	2.20958	–0.73693	0.00000
O	–0.31967	3.08150	0.00000
N	2.36385	4.68960	0.00000
C	3.66098	4.74781	0.00000
N	4.25201	3.50135	0.00000
H	0.16707	0.69456	0.00000
H	1.35738	–1.28448	0.00000
H	3.09425	–1.21079	0.00000
H	5.23442	3.28561	0.00000
H	4.25014	5.65301	0.00000

Sum of electronic and zero–point Energies: –1084.853435 a.u.
N_{Im}= 2 (305*i* cm^{-1}, 16*i* cm^{-1})

G•6-thioG 3

	X	Y	Z
N	–2.43396	–3.78962	0.00000
C	–1.40936	–2.84222	0.00000
C	–1.93582	–1.53269	0.00000
C	–3.31495	–1.36031	0.00000
N	–4.27003	–2.30935	0.00000
C	–3.77701	–3.52064	0.00000
N	–4.61696	–4.58268	0.00000
S	0.17601	–3.34102	0.00000
N	–1.30549	–0.30898	0.00000
C	–2.26250	0.57425	0.00000
N	–3.50670	–0.01190	0.00000
H	–2.11233	–4.74829	0.00000
H	–4.29671	–5.53301	0.00000
H	–5.60369	–4.39509	0.00000
H	–4.39636	0.45950	0.00000
H	–2.09156	1.64463	0.00000
N	1.15927	1.21995	0.00000
C	0.83807	2.59236	0.00000
C	2.03095	3.38695	0.00000
C	3.25390	2.73277	0.00000
N	3.51449	1.40890	0.00000
C	2.41651	0.68754	0.00000
N	2.49936	–0.66019	0.00000
O	–0.33135	2.94323	0.00000
N	2.20394	4.75595	0.00000
C	3.49141	4.92279	0.00000
N	4.18570	3.73039	0.00000
H	0.35441	0.58092	0.00000
H	1.68774	–1.26519	0.00000
H	3.41714	–1.06639	0.00000

H	5.18291	3.59842	0.00000
H	4.00232	5.87432	0.00000

Sum of electronic and zero–point Energies: –1407.816862 a.u.
N_{Im}= 2 (283*i* cm^{-1}, 3*i* cm^{-1})

6-thioG•G 3

	X	Y	Z
N	–2.09249	–3.76034	0.00000
C	–1.21210	–2.65466	0.00000
C	–1.94715	–1.43498	0.00000
C	–3.32832	–1.48267	0.00000
N	–4.13086	–2.57031	0.00000
C	–3.46354	–3.69217	0.00000
N	–4.13667	–4.86842	0.00000
O	–0.00691	–2.83631	0.00000
N	–1.50336	–0.13236	0.00000
C	–2.58511	0.59339	0.00000
N	–3.72332	–0.17677	0.00000
H	–1.62762	–4.65729	0.00000
H	–3.67908	–5.76052	0.00000
H	–5.14031	–4.82921	0.00000
H	–4.67455	0.15296	0.00000
H	–2.58628	1.67524	0.00000
N	1.03331	1.34059	0.00000
C	0.95011	2.72747	0.00000
C	2.23533	3.32387	0.00000
C	3.35008	2.49080	0.00000
N	3.39209	1.14922	0.00000
C	2.18997	0.61012	0.00000
N	2.07255	–0.73167	0.00000
S	–0.52618	3.50562	0.00000
N	2.62052	4.65001	0.00000
C	3.91633	4.61614	0.00000
N	4.42363	3.33083	0.00000
H	0.14135	0.82770	0.00000
H	1.19607	–1.24150	0.00000
H	2.92828	–1.25677	0.00000
H	5.38928	3.04890	0.00000
H	4.56691	5.47839	0.00000

Sum of electronic and zero–point Energies: –1407.817632 a.u.
N_{Im}= 2 (296*i* cm^{-1}, 9*i* cm^{-1})

G•A 2

	X	Y	Z
N	–3.24620	1.71991	0.00000
C	–4.44997	0.95392	0.00000
C	–4.13001	–0.44604	0.00000
C	–2.79792	–0.82136	0.00000
N	–1.68714	–0.04261	0.00000
C	–1.96276	1.24266	0.00000

N	–0.96647	2.14714	0.00000
O	–5.51410	1.52590	0.00000
N	–4.95467	–1.54945	0.00000
C	–4.14574	–2.56360	0.00000
N	–2.81782	–2.18572	0.00000
H	–3.40857	2.71669	0.00000
H	–1.16622	3.13021	0.00000
H	0.01076	1.83935	0.00000
H	–2.01676	–2.79324	0.00000
H	–4.43688	–3.60340	0.00000
C	4.47305	–1.60576	0.00000
N	3.19720	–1.99948	0.00000
C	2.22695	–1.07338	0.00000
C	2.61015	0.28452	0.00000
N	4.95797	–0.36964	0.00000
C	3.97661	0.53164	0.00000
N	4.08841	1.90041	0.00000
N	1.90105	1.47313	0.00000
C	2.81745	2.40209	0.00000
H	4.95048	2.41996	0.00000
N	0.95136	–1.48645	0.00000
H	2.62598	3.46501	0.00000
H	5.20676	–2.40624	0.00000
H	0.14793	–0.85747	0.00000
H	0.81026	–2.48221	0.00000

Sum of electronic and zero–point Energies: –1009.604372 a.u.
N_{Im}= 2 (132*i* cm^{-1}, 26*i* cm^{-1})

G•A 4

	X	Y	Z
N	1.30907	–1.95676	0.00000
C	2.55290	–1.25741	0.00000
C	2.31069	0.15824	0.00000
C	1.00124	0.60573	0.00000
N	–0.14958	–0.11081	0.00000
C	0.05298	–1.41140	0.00000
N	–0.99256	–2.25672	0.00000
O	3.58434	–1.88653	0.00000
N	3.19393	1.21564	0.00000
C	2.44112	2.27219	0.00000
N	1.09447	1.96693	0.00000
H	1.41641	–2.96101	0.00000
H	–0.84987	–3.24984	0.00000
H	–1.95274	–1.88830	0.00000
H	0.32564	2.61525	0.00000
H	2.78856	3.29456	0.00000
C	–4.78225	–2.06875	0.00000
N	–3.73926	–1.22462	0.00000
C	–3.97182	0.10003	0.00000
C	–5.31430	0.52748	0.00000

N	–6.07357	–1.78628	0.00000
C	–6.28197	–0.46506	0.00000
N	–7.47306	0.21182	0.00000
N	–5.88321	1.78448	0.00000
C	–7.16446	1.55091	0.00000
H	–8.38952	–0.20419	0.00000
N	–2.94460	0.95688	0.00000
H	–7.93524	2.30765	0.00000
H	–4.52374	–3.12396	0.00000
H	–3.14831	1.94141	0.00000
H	–1.97868	0.61937	0.00000

Sum of electronic and zero–point Energies: –1009.606570 a.u.
N_{Im}= 2 (83*i* cm^{-1}, 9*i* cm^{-1})

A•A 1

	X	Y	Z
C	0.71943	1.10376	0.00000
N	–0.02987	–0.00777	0.00000
C	0.58003	–1.20785	0.00000
C	1.99042	–1.22122	0.00000
N	2.03783	1.21409	0.00000
C	2.62384	0.01156	0.00000
N	3.96179	–0.28551	0.00000
N	2.90428	–2.25557	0.00000
C	4.06028	–1.65632	0.00000
H	4.71493	0.38185	0.00000
N	–0.15021	–2.32624	0.00000
H	5.01939	–2.15327	0.00000
H	0.16245	2.03667	0.00000
H	0.32982	–3.20972	0.00000
H	–1.17544	–2.28938	0.00000
C	–3.86209	–3.27949	0.00000
N	–3.11282	–2.16794	0.00000
C	–3.72274	–0.96788	0.00000
C	–5.13313	–0.95454	0.00000
N	–5.18049	–3.38985	0.00000
C	–5.76652	–2.18734	0.00000
N	–7.10448	–1.89029	0.00000
N	–6.04701	0.07979	0.00000
C	–7.20300	–0.51949	0.00000
H	–7.85760	–2.55767	0.00000
N	–2.99252	0.15052	0.00000
H	–8.16212	–0.02256	0.00000
H	–3.30509	–4.21239	0.00000
H	–3.47255	1.03400	0.00000
H	–1.96729	0.11367	0.00000

Sum of electronic and zero–point Energies: –934.371116 a.u.
N_{Im}= 0

A•A 2

	X	Y	Z
C	–2.11535	–1.82280	0.00000
N	–1.22146	–0.82372	0.00000
C	–1.66382	0.44587	0.00000
C	–3.05861	0.65219	0.00000
N	–3.43655	–1.75341	0.00000
C	–3.85410	–0.48286	0.00000
N	–5.13916	–0.00647	0.00000
N	–3.82310	1.80142	0.00000
C	–5.05002	1.36484	0.00000
H	–5.97623	–0.56502	0.00000
N	–0.78844	1.45560	0.00000
H	–5.93252	1.98774	0.00000
H	–1.69085	–2.82318	0.00000
H	–1.14388	2.39598	0.00000
H	0.21936	1.28035	0.00000
C	5.03516	–1.72933	0.00000
N	3.80778	–2.25288	0.00000
C	2.74473	–1.43169	0.00000
C	2.98879	–0.04006	0.00000
N	5.39224	–0.44989	0.00000
C	4.32239	0.34570	0.00000
N	4.29383	1.71880	0.00000
N	2.16155	1.06990	0.00000
C	2.97719	2.08765	0.00000
H	5.09827	2.32336	0.00000
N	1.51980	–1.96955	0.00000
H	2.67704	3.12520	0.00000
H	5.84757	–2.45021	0.00000
H	0.65624	–1.42177	0.00000
H	1.46832	–2.97420	0.00000

Sum of electronic and zero–point Energies: –934.369613 a.u.
N_{Im}= 1 (4*i* cm^{-1})

A•A 3

	X	Y	Z
C	–2.67838	–0.37540	0.00000
N	–1.82569	–1.40284	0.00000
C	–0.50647	–1.15603	0.00000
C	–0.08579	0.19099	0.00000
N	–2.41024	0.92514	0.00000
C	–1.09506	1.14446	0.00000
N	–0.44036	2.35127	0.00000
N	1.15849	0.79581	0.00000
C	0.89917	2.07400	0.00000
H	–0.87728	3.25779	0.00000
N	0.34066	–2.19322	0.00000
H	1.64094	2.85931	0.00000
H	–3.73045	–0.64493	0.00000
H	1.35489	–2.09353	0.00000

H	–0.06862	–3.11175	0.00000
C	7.14017	–1.41077	0.00000
N	6.28747	–0.38333	0.00000
C	4.96826	–0.63014	0.00000
C	4.54757	–1.97716	0.00000
N	6.87202	–2.71132	0.00000
C	5.55685	–2.93063	0.00000
N	4.90215	–4.13744	0.00000
N	3.30330	–2.58198	0.00000
C	3.56261	–3.86017	0.00000
H	5.33906	–5.04396	0.00000
N	4.12113	0.40705	0.00000
H	2.82085	–4.64548	0.00000
H	8.19224	–1.14124	0.00000
H	3.10690	0.30736	0.00000
H	4.53041	1.32558	0.00000

Sum of electronic and zero–point Energies: –934.367134 a.u.
N_{Im}= 1 (17*i* cm^{-1})

8-oxoG•G

	X	Y	Z
N	–2.65435	0.77097	0.00000
C	–2.55469	–0.62797	0.00000
C	–3.85293	–1.22890	0.00000
C	–4.95954	–0.39084	0.00000
N	–5.00809	0.95909	0.00000
C	–3.81131	1.49246	0.00000
N	–3.66462	2.83882	0.00000
O	–1.45009	–1.15761	0.00000
N	–4.23767	–2.55309	0.00000
C	–5.53493	–2.51606	0.00000
N	–6.03480	–1.22964	0.00000
H	–1.76577	1.29153	0.00000
H	–2.75294	3.26364	0.00000
H	–4.49184	3.40639	0.00000
H	–6.99955	–0.94427	0.00000
H	–6.18823	–3.37600	0.00000
C	3.02594	–1.13579	0.00000
C	2.29127	0.08213	0.00000
N	0.92435	0.34667	0.00000
C	0.72660	1.69088	0.00000
N	1.99099	2.26306	0.00000
C	2.95277	1.28348	0.00000
N	4.28372	1.50239	0.00000
C	4.98551	0.39850	0.00000
N	4.42361	–0.84423	0.00000
N	6.33988	0.47441	0.00000
O	–0.33645	2.31395	0.00000
H	0.14499	–0.33000	0.00000
H	5.00485	–1.67046	0.00000

H	6.93067	–0.33554	0.00000
H	6.75449	1.38896	0.00000
O	2.64921	–2.28659	0.00000
H	2.15122	3.25590	0.00000

Sum of electronic and zero–point Energies: –1160.103732 a.u.
N_{Im}= 2 (313*i* cm^{-1}, 156*i* cm^{-1})

2-thioU•2-thioU

	X	Y	Z
C	–3.51513	–1.17386	0.00000
C	2.81952	0.89735	0.00000
O	–3.30742	–2.36257	0.00000
S	3.07026	2.53127	0.00000
N	–2.44005	–0.25847	0.00000
N	1.58779	0.30993	0.00000
C	–2.52635	1.09196	0.00000
C	1.30376	–1.05275	0.00000
N	–3.80248	1.58540	0.00000
C	2.46894	–1.91696	0.00000
C	–4.83013	–0.54373	0.00000
N	3.85892	–0.00171	0.00000
C	–4.92281	0.79319	0.00000
C	3.69109	–1.35947	0.00000
H	–1.49775	–0.67341	0.00000
H	0.77168	0.93400	0.00000
S	–1.22627	2.14265	0.00000
O	0.14866	–1.44251	0.00000
H	–3.87890	2.59030	0.00000
H	2.32024	–2.98566	0.00000
H	–5.70204	–1.17998	0.00000
H	4.78062	0.40633	0.00000
H	–5.86643	1.32361	0.00000
H	4.60418	–1.94102	0.00000

Sum of electronic and zero–point Energies: –1475.365216 a.u.
N_{Im}= 0

T•T 1

	X	Y	Z
C	–1.78388	1.35305	0.00000
C	1.67113	–0.80299	0.00000
O	–1.77577	0.13131	0.00000
O	1.61802	0.41957	0.00000
N	–0.65848	2.12791	0.00000
N	0.51435	–1.56268	0.00000
C	–0.60514	3.52634	0.00000
C	0.42837	–2.94004	0.00000
C	–1.91181	4.19950	0.00000
N	1.66550	–3.56335	0.00000
N	–2.96190	2.06125	0.00000

C	2.93004	–1.54533	0.00000
C	–3.01659	3.43830	0.00000
C	2.86052	–2.88770	0.00000
H	0.23287	1.61333	0.00000
H	–0.37402	–1.04408	0.00000
O	0.45764	4.10602	0.00000
O	–0.61019	–3.55657	0.00000
C	–1.92692	5.69548	0.00000
H	1.63820	–4.56985	0.00000
H	–3.80119	1.50510	0.00000
C	4.21015	–0.76993	0.00000
H	–4.01459	3.85983	0.00000
H	3.74596	–3.51243	0.00000
H	5.07242	–1.43978	0.00000
H	4.26907	–0.12136	–0.87730
H	4.26907	–0.12136	0.87730
H	–2.94954	6.07812	0.00000
H	–1.40478	6.08495	0.87728
H	–1.40478	6.08495	–0.87728

Sum of electronic and zero–point Energies: –908.031924 a.u.
N_{Im}= 0

T•T 2

	X	Y	Z
C	–1.78204	1.37339	0.00000
C	1.62204	–0.80339	0.00000
O	–1.77452	0.15222	0.00000
O	1.61452	0.41778	0.00000
N	–0.65611	2.14838	0.00000
N	0.49611	–1.57838	0.00000
C	–0.60123	3.54671	0.00000
C	0.44123	–2.97671	0.00000
C	–1.90706	4.22086	0.00000
C	1.74706	–3.65086	0.00000
N	–2.95922	2.08330	0.00000
N	2.79922	–1.51330	0.00000
C	–3.01245	3.46031	0.00000
C	2.85245	–2.89031	0.00000
H	0.23435	1.63495	0.00000
H	–0.39435	–1.06495	0.00000
O	0.46266	4.12461	0.00000
O	–0.62266	–3.55461	0.00000
C	–1.92107	5.71688	0.00000
C	1.76107	–5.14688	0.00000
H	–3.79917	1.52808	0.00000
H	3.63917	–0.95808	0.00000
H	–4.01000	3.88287	0.00000
H	3.85000	–3.31287	0.00000
H	2.78340	–5.53025	0.00000
H	1.23873	–5.53603	0.87732

H	1.23873	–5.53603	–0.87732
H	–2.94340	6.10025	0.00000
H	–1.39873	6.10603	0.87732
H	–1.39873	6.10603	–0.87732

Sum of electronic and zero–point Energies: –908.031449 a.u.
N_{Im}= 0

T•T 3

	X	Y	Z
C	–3.57886	–1.22315	0.00000
C	2.53886	0.95315	0.00000
O	–3.62430	–2.42991	0.00000
O	2.58430	2.15991	0.00000
N	–2.41042	–0.48868	0.00000
N	1.37042	0.21868	0.00000
C	–2.29783	0.89008	0.00000
C	1.25783	–1.16008	0.00000
C	–3.55160	1.64081	0.00000
C	2.51160	–1.91081	0.00000
N	–4.71838	–0.43478	0.00000
N	3.67838	0.16478	0.00000
C	–4.69714	0.93758	0.00000
C	3.65714	–1.20758	0.00000
H	–1.52806	–1.02006	0.00000
H	0.48806	0.75006	0.00000
O	–1.19869	1.42927	0.00000
O	0.15869	–1.69927	0.00000
C	–3.48294	3.13588	0.00000
C	2.44294	–3.40588	0.00000
H	–5.58900	–0.94057	0.00000
H	4.54900	0.67057	0.00000
H	–5.66939	1.41617	0.00000
H	4.62939	–1.68617	0.00000
H	3.44362	–3.84277	0.00000
H	1.90156	–3.76783	0.87732
H	1.90156	–3.76783	–0.87732
H	–4.48362	3.57277	0.00000
H	–2.94156	3.49783	0.87732
H	–2.94156	3.49783	–0.87732

Sum of electronic and zero–point Energies: –908.032435 a.u.
N_{Im}= 0

T•C 1

	X	Y	Z
C	–2.21645	–1.19283	0.00000
N	–1.58091	–0.03182	0.00000
C	–2.28285	1.14404	0.00000
O	–1.78565	2.24705	0.00000
N	–3.69429	1.03781	0.00000
C	–4.34910	–0.14481	0.00000

C	–3.65451	–1.30064	0.00000
N	–1.48214	–2.31279	0.00000
H	–5.43161	–0.10494	0.00000
H	–4.15190	–2.25963	0.00000
H	–0.46223	–2.24910	0.00000
H	–1.92737	–3.21190	0.00000
H	–4.18922	1.91554	0.00000
C	1.98785	–1.00974	0.00000
O	1.32707	–2.04002	0.00000
N	1.46028	0.24926	0.00000
C	2.18859	1.45217	0.00000
C	3.65331	1.29863	0.00000
N	3.36157	–1.06025	0.00000
C	4.16452	0.06033	0.00000
H	0.42887	0.30881	0.00000
O	1.63011	2.52160	0.00000
C	4.47989	2.54532	0.00000
H	3.75726	–1.98557	0.00000
H	5.23031	–0.13418	0.00000
H	5.54624	2.30998	0.00000
H	4.25253	3.15629	–0.87688
H	4.25253	3.15629	0.87688

Sum of electronic and zero–point Energies: –848.841605 a.u.
N_{Im}= 1 (27*i* cm^{-1})

T•C 2

	X	Y	Z
C	0.15991	0.12779	0.00000
O	–0.39990	1.19290	0.00000
N	–0.47795	–1.10222	0.00000
C	0.13574	–2.34084	0.00000
C	1.59698	–2.34916	0.00000
N	1.54625	0.02508	0.00000
C	2.22750	–1.16234	0.00000
H	–1.51212	–1.09154	0.00000
O	–0.52277	–3.37514	0.00000
C	2.29950	–3.67093	0.00000
H	2.03451	0.90560	0.00000
H	3.30823	–1.08022	0.00000
H	3.38316	–3.53593	0.00000
H	2.02029	–4.25859	0.87797
H	2.02029	–4.25859	–0.87797
C	–4.08761	–2.65301	0.00000
N	–3.49625	–1.46824	0.00000
C	–4.24148	–0.31968	0.00000
O	–3.78599	0.80143	0.00000
N	–5.64780	–0.47862	0.00000
C	–6.25798	–1.68503	0.00000
C	–5.52078	–2.81407	0.00000
N	–3.31133	–3.74345	0.00000

H	–7.34122	–1.68561	0.00000
H	–5.98193	–3.79100	0.00000
H	–2.29334	–3.64019	0.00000
H	–3.72209	–4.65887	0.00000
H	–6.17523	0.37993	0.00000

Sum of electronic and zero–point Energies: –848.842583 a.u.
N_{Im}= 1 (26*i* cm^{-1})

I•I

	X	Y	Z
N	–1.54032	–1.01498	0.00000
N	1.52819	1.02636	0.00000
C	–2.01586	0.30119	0.00000
C	2.00375	–0.28981	0.00000
C	–3.44874	0.32362	0.00000
C	3.43663	–0.31223	0.00000
C	–4.12669	–0.88602	0.00000
C	4.11457	0.89741	0.00000
N	–3.61232	–2.13871	0.00000
N	3.60019	2.15010	0.00000
C	–2.31378	–2.12844	0.00000
C	2.30164	2.13982	0.00000
H	–1.77234	–3.06812	0.00000
H	1.76019	3.07949	0.00000
O	–1.23754	1.24986	0.00000
O	1.22544	–1.23849	0.00000
N	–4.32939	1.37978	0.00000
N	4.31729	–1.36838	0.00000
C	–5.50500	0.82183	0.00000
C	5.49290	–0.81043	0.00000
N	–5.44913	–0.55148	0.00000
N	5.43701	0.56289	0.00000
H	–0.51013	–1.12681	0.00000
H	0.49800	1.13817	0.00000
H	–6.21959	–1.19942	0.00000
H	6.20746	1.21083	0.00000
H	–6.44718	1.34979	0.00000
H	6.43508	–1.33838	0.00000

Sum of electronic and zero–point Energies: –974.142867 a.u.
N_{Im}= 0

G*•T

	X	Y	Z
C	–0.59335	1.04013	0.00000
C	3.61805	–1.21135	0.00000
N	0.15572	–0.09748	0.00000
N	3.01328	0.03025	0.00000
C	–0.45820	–1.28234	0.00000
C	3.64609	1.24546	0.00000
C	–1.85938	–1.32879	0.00000

N	5.02105	1.16045	0.00000
N	–1.92462	1.11210	0.00000
C	5.07810	–1.22216	0.00000
C	–2.49433	–0.08949	0.00000
C	5.70465	–0.03270	0.00000
N	–3.82928	–0.38257	0.00000
N	–2.78117	–2.36149	0.00000
C	–3.93017	–1.76110	0.00000
O	0.23517	–2.39613	0.00000
H	–4.89177	–2.25347	0.00000
N	0.08319	2.21021	0.00000
O	2.93537	–2.22835	0.00000
H	1.96702	0.03462	0.00000
O	3.06034	2.31200	0.00000
H	6.78452	0.05347	0.00000
H	–4.57918	0.28776	0.00000
H	5.51117	2.04039	0.00000
C	5.78055	–2.54335	0.00000
H	–0.45698	3.05593	0.00000
H	1.09470	2.25836	0.00000
H	1.20746	–2.24363	0.00000
H	6.86400	–2.41022	0.00000
H	5.49843	–3.12945	0.87775
H	5.49843	–3.12945	–0.87775

Sum of electronic and zero–point Energies: –996.444910 a.u.
N_{Im}= 1 (13*i* cm^{-1})

6-thioG•C

	X	Y	Z
C	0.17633	1.42454	0.00000
N	0.05455	0.09813	0.00000
C	1.16079	–0.68377	0.00000
O	1.13918	–1.91027	0.00000
N	2.41064	–0.05448	0.00000
C	2.55082	1.29397	0.00000
C	1.45930	2.08271	0.00000
N	–0.93437	2.15524	0.00000
C	–3.86911	–0.76743	0.00000
C	–4.97667	–1.64252	0.00000
C	–4.73501	–3.01344	0.00000
N	–3.55713	–3.64866	0.00000
C	–2.52973	–2.82048	0.00000
N	–2.66275	–1.45153	0.00000
S	–3.94174	0.90521	0.00000
N	–1.28564	–3.31674	0.00000
N	–6.33463	–1.38735	0.00000
C	–6.88731	–2.55905	0.00000
N	–5.96841	–3.59242	0.00000
H	3.56273	1.67877	0.00000
H	1.54132	3.15981	0.00000

H	–1.20847	–4.31812	0.00000
H	–0.43552	–2.74682	0.00000
H	–7.95020	–2.75138	0.00000
H	–1.85937	1.70062	0.00000
H	–0.88506	3.15850	0.00000
H	–1.80490	–0.88788	0.00000
H	3.20884	–0.66976	0.00000
H	–6.15282	–4.58149	0.00000

Sum of electronic and zero–point Energies: –1260.231077 a.u.
N_{Im}= 1 (15*i* cm^{-1})

8-oxoG•C

	X	Y	Z
C	0.02001	1.34401	0.00000
N	–0.00168	0.01335	0.00000
C	1.14609	–0.70584	0.00000
O	1.18773	–1.93045	0.00000
N	2.35110	0.00561	0.00000
C	2.39750	1.36159	0.00000
C	1.25803	2.08174	0.00000
N	–1.14562	1.98583	0.00000
C	–3.61244	–0.71351	0.00000
C	–4.77886	–1.49455	0.00000
C	–4.68328	–2.86899	0.00000
N	–3.56578	–3.60512	0.00000
C	–2.46120	–2.87802	0.00000
N	–2.46518	–1.51368	0.00000
O	–3.52198	0.52210	0.00000
N	–1.26252	–3.48472	0.00000
N	–6.13511	–1.16797	0.00000
C	–6.90096	–2.31107	0.00000
N	–5.96519	–3.35567	0.00000
H	3.38171	1.81271	0.00000
H	1.27460	3.16185	0.00000
H	–1.26067	–4.48868	0.00000
H	–0.38331	–2.96736	0.00000
O	–8.10617	–2.41732	0.00000
H	–2.03410	1.45859	0.00000
H	–1.16804	2.98995	0.00000
H	–1.56692	–1.00224	0.00000
H	3.19121	–0.55132	0.00000
H	–6.22999	–4.32577	0.00000
H	–6.52636	–0.24307	0.00000

Sum of electronic and zero–point Energies: –1012.524863 a.u.
N_{Im}= 0

2-aminoA•T

	X	Y	Z
C	–0.63279	1.05384	0.00000
C	3.67664	–1.27848	0.00000

N	0.10165	–0.09196	0.00000
N	3.01980	–0.05656	0.00000
C	–0.53989	–1.27038	0.00000
C	3.61305	1.17942	0.00000
C	–1.94840	–1.27095	0.00000
N	4.99037	1.14774	0.00000
N	–1.96583	1.16100	0.00000
C	5.13921	–1.22649	0.00000
C	–2.56093	–0.02945	0.00000
C	5.72141	–0.01627	0.00000
N	–3.90260	–0.30777	0.00000
N	–2.87766	–2.29527	0.00000
C	–4.02384	–1.68283	0.00000
N	0.15515	–2.41525	0.00000
H	–4.99089	–2.16376	0.00000
N	0.06316	2.21178	0.00000
O	3.04723	–2.32476	0.00000
H	–0.35667	–3.28039	0.00000
H	1.17192	–2.42359	0.00000
H	1.97385	–0.06825	0.00000
O	2.99767	2.22955	0.00000
C	5.89226	–2.51949	0.00000
H	6.96987	–2.34451	0.00000
H	5.63313	–3.11628	0.87774
H	5.63313	–3.11628	–0.87774
H	6.79715	0.11202	0.00000
H	–4.64497	0.37083	0.00000
H	5.44286	2.04739	0.00000
H	–0.46184	3.06673	0.00000
H	1.07552	2.23374	0.00000

Sum of electronic and zero–point Energies: –976.569244 a.u.
N_{Im}= 1 (25*i* cm^{-1})

A•T(Hoog')

	X	Y	Z
C	–1.19011	–2.04405	0.00000
C	0.04691	–1.37808	0.00000
N	1.35016	–1.82616	0.00000
C	2.05586	–0.72676	0.00000
N	1.30122	0.41620	0.00000
C	0.00052	0.00918	0.00000
N	–1.11498	0.75736	0.00000
C	–2.21623	0.01204	0.00000
N	–2.31615	–1.31660	0.00000
N	–1.28156	–3.38576	0.00000
O	0.21288	7.51242	0.00000
C	–0.10804	6.34390	0.00000
N	0.87381	5.34308	0.00000
C	0.68251	3.98340	0.00000
O	1.62410	3.19897	0.00000

N	–0.62632	3.60108	0.00000
C	–1.65969	4.50658	0.00000
C	–1.48042	5.83990	0.00000
C	–2.59624	6.83721	0.00000
H	–2.18952	–3.81602	0.00000
H	–0.44840	–3.94746	0.00000
H	–3.15928	0.55081	0.00000
H	1.60482	1.39626	0.00000
H	3.13512	–0.68553	0.00000
H	1.83500	5.65566	0.00000
H	–0.83342	2.58617	0.00000
H	–2.64733	4.06026	0.00000
H	–3.56698	6.33775	0.00000
H	–2.53488	7.48518	–0.87778
H	–2.53488	7.48518	0.87778

Sum of electronic and zero–point Energies: –921.211160 a.u.
N_{Im}= 0

3. Acyclic references

1

	X	Y	Z
N	0.18923	–0.48124	0.00000
C	–0.20128	–1.79172	0.00000
C	–0.63386	0.66059	0.00000
N	0.10905	1.82100	0.00000
O	0.58255	–2.70988	0.00000
H	–0.35853	2.70727	0.00000
H	1.11075	1.81963	0.00000
H	–1.29038	–1.93584	0.00000
H	1.19083	–0.35377	0.00000
C	–1.97454	0.64017	0.00000
H	–2.52108	1.57305	0.00000
H	–2.54570	–0.27376	0.00000

Sum of electronic and zero–point Energies: –302.536089 a.u.
N_{Im}= 2 (490*i* cm^{-1}, 200*i* cm^{-1})

2

	X	Y	Z
N	1.57780	0.98327	0.00000
C	1.93137	–0.33839	0.00000
C	2.42918	2.09364	0.00000
H	1.87945	3.02837	0.00000
O	1.12917	–1.24020	0.00000
H	0.58280	1.15161	0.00000
H	3.01846	–0.50815	0.00000
C	3.75978	2.10942	0.00000
H	4.26858	3.06347	0.00000
H	4.37646	1.22009	0.00000

Sum of electronic and zero–point Energies: –247.193935 a.u.

N_{Im}= 1 (100*i* cm^{-1})

3

	X	Y	Z
C	0.20494	–0.64054	0.00000
N	–0.30183	–1.88119	0.00000
N	–0.54054	0.40529	0.00000
C	0.15211	1.61196	0.00000
O	–0.37064	2.69133	0.00000
H	0.29021	–2.69133	0.00000
H	–1.30224	–1.99980	0.00000
H	1.26514	1.52036	0.00000
H	1.30224	–0.59637	0.00000

Sum of electronic and zero–point Energies: –263.259242 a.u.
N_{Im}= 0

4

	X	Y	Z
C	2.52950	0.93984	0.00000
O	2.59986	2.13711	0.00000
N	1.33685	0.24126	0.00000
C	1.24181	–1.13766	0.00000
H	0.47573	0.77500	0.00000
O	0.20084	–1.73328	0.00000
H	3.41334	0.27933	0.00000
H	2.22657	–1.63537	0.00000

Sum of electronic and zero–point Energies: –283.161275 a.u.
N_{Im}= 0

5

	X	Y	Z
C	2.44238	2.14995	0.00000
N	1.61902	1.01280	0.00000
C	2.13137	–0.15484	0.00000
N	1.36179	–1.26910	0.00000
H	1.85938	3.06684	0.00000
H	1.76685	–2.18593	0.00000
H	0.36039	–1.16848	0.00000
H	3.20611	–0.36685	0.00000
C	3.77441	2.24825	0.00000
H	4.23676	3.22721	0.00000
H	4.44522	1.39551	0.00000

Sum of electronic and zero–point Energies: –227.291863 a.u.
N_{Im}= 2 (226*i* cm^{-1}, 138*i* cm^{-1})

6

	X	Y	Z
C	1.36079	1.19382	0.00000
N	0.54164	2.27188	0.00000
N	0.90475	0.00583	0.00000

C	1.78394	–1.09770	0.00000
N	1.04913	–2.25993	0.00000
C	3.13093	–1.07890	0.00000
H	0.90769	3.20491	0.00000
H	–0.45452	2.13073	0.00000
H	2.42441	1.44903	0.00000
H	1.49140	–3.15873	0.00000
H	0.04918	–2.19131	0.00000
H	3.69267	–2.00404	0.00000
H	3.69932	–0.16055	0.00000

Sum of electronic and zero–point Energies: –282.641376 a.u.
N_{Im}= 3 (393*i* cm^{-1}, 160*i* cm^{-1}, 131*i* cm^{-1})

1•1

	X	Y	Z
C	0.30964	0.45144	0.00000
O	–0.47457	1.39422	0.00000
N	–3.28095	0.83145	0.00000
C	–3.67558	–0.45144	0.00000
C	–4.09436	1.98558	0.00000
N	–3.31444	3.11580	0.00000
O	–2.89137	–1.39422	0.00000
H	–2.26709	0.99217	0.00000
N	–0.08499	–0.83145	0.00000
C	0.72842	–1.98558	0.00000
H	–1.09885	–0.99217	0.00000
N	–0.05149	–3.11580	0.00000
H	–3.74796	4.01890	0.00000
H	–2.31041	3.06228	0.00000
H	0.38202	–4.01890	0.00000
H	–1.05552	–3.06228	0.00000
H	–4.75955	–0.61511	0.00000
H	1.39361	0.61511	0.00000
C	2.06966	–1.98215	0.00000
H	2.60681	–2.92043	0.00000
H	2.65047	–1.07359	0.00000
C	–5.43559	1.98215	0.00000
H	–5.97275	2.92043	0.00000
H	–6.01640	1.07359	0.00000

Sum of electronic and zero–point Energies: –605.103357 a.u.
N_{Im}= 4 (345*i* cm^{-1}, 339*i* cm^{-1}, 129*i* cm^{-1}, 103*i* cm^{-1})

2•2

	X	Y	Z
N	–1.62436	–0.94032	0.00000
N	1.61223	0.95170	0.00000
C	–2.01286	0.35094	0.00000
C	2.00074	–0.33956	0.00000
C	–2.45988	–2.06454	0.00000
C	2.44774	2.07592	0.00000

H	–1.88831	–2.98574	0.00000
H	1.87617	2.99712	0.00000
O	–1.23867	1.29625	0.00000
O	1.22655	–1.28487	0.00000
H	–0.61142	–1.10546	0.00000
H	0.59929	1.11683	0.00000
H	–3.09957	0.51077	0.00000
C	–3.78989	–2.10548	0.00000
H	–4.28139	–3.06866	0.00000
H	–4.42466	–1.22847	0.00000
H	3.08744	–0.49939	0.00000
C	3.77776	2.11688	0.00000
H	4.26925	3.08006	0.00000
H	4.41254	1.23986	0.00000

Sum of electronic and zero–point Energies: –494.410697 a.u.
N_{Im}= 2 (89*i* cm^{-1}, 82*i* cm^{-1})

3•3

	X	Y	Z
C	4.21314	0.07064	0.00000
N	3.68401	–1.13849	0.00000
N	0.79179	–1.16081	0.00000
C	0.06616	–0.07899	0.00000
C	0.10343	–2.35705	0.00000
O	0.64086	–3.43519	0.00000
N	0.59529	1.13014	0.00000
N	3.48751	1.15246	0.00000
C	4.17587	2.34870	0.00000
O	3.63844	3.42684	0.00000
H	4.27135	–1.95383	0.00000
H	2.65474	–1.24906	0.00000
H	0.00795	1.94548	0.00000
H	1.62456	1.24071	0.00000
H	–1.00771	–2.27398	0.00000
H	5.28701	2.26563	0.00000
H	–1.02964	–0.12671	0.00000
H	5.30894	0.11836	0.00000

Sum of electronic and zero–point Energies: –526.552057 a.u.
N_{Im}= 0

4•4

	X	Y	Z
C	–3.63671	–1.21296	0.00000
C	2.59671	0.94296	0.00000
O	–3.74892	–2.40513	0.00000
O	2.70892	2.13513	0.00000
N	–2.41896	–0.55016	0.00000
N	1.37896	0.28016	0.00000
C	–2.32238	0.81118	0.00000
C	1.28238	–1.08118	0.00000

H	–1.54795	–1.09547	0.00000
H	0.50795	0.82547	0.00000
O	–1.27726	1.42247	0.00000
O	0.23726	–1.69247	0.00000
H	–3.29531	1.32827	0.00000
H	–4.50005	–0.52386	0.00000
H	3.46005	0.25386	0.00000
H	2.25531	–1.59827	0.00000

Sum of electronic and zero–point Energies: –566.339759 a.u.
N_{Im}= 0

5•5

	X	Y	Z
C	–2.85142	1.50698	0.00000
N	–1.77025	0.61474	0.00000
C	–1.98151	–0.65731	0.00000
N	–0.99025	–1.55394	0.00000
H	–2.51853	2.54235	0.00000
H	–1.21200	–2.53260	0.00000
H	0.00000	–1.25431	0.00000
C	2.85142	–1.50698	0.00000
N	1.77024	–0.61473	0.00000
C	1.98150	0.65731	0.00000
N	0.99025	1.55394	0.00000
H	2.51852	–2.54234	0.00000
H	1.21200	2.53260	0.00000
H	0.00000	1.25431	0.00000
H	2.98646	1.09048	0.00000
C	4.16761	–1.27644	0.00000
H	4.85342	–2.11383	0.00000
H	4.61083	–0.28667	0.00000
H	–2.98646	–1.09048	0.00000
C	–4.16761	1.27644	0.00000
H	–4.85343	2.11383	0.00000
H	–4.61083	0.28667	0.00000

Sum of electronic and zero–point Energies: –454.606657 a.u.
N_{Im}= 2 (186*i* cm^{-1}, 181*i* cm^{-1})

3•1

	X	Y	Z
C	3.68235	–2.88165	0.00000
O	3.00743	–3.88501	0.00000
N	0.24392	–1.16091	0.00000
C	–0.04398	0.14888	0.00000
C	–0.67582	–2.23523	0.00000
N	–0.02479	–3.43940	0.00000
O	0.80694	1.03324	0.00000
H	1.24673	–1.38925	0.00000
N	3.14590	–1.61750	0.00000
C	3.98746	–0.62402	0.00000

N	3.58606	0.63343	0.00000
H	–0.56854	–4.28133	0.00000
H	0.98373	–3.53052	0.00000
H	4.25748	1.38086	0.00000
H	2.57504	0.84720	0.00000
H	–1.11131	0.39921	0.00000
H	4.79207	–2.95001	0.00000
C	–2.01228	–2.09155	0.00000
H	–2.64180	–2.97071	0.00000
H	–2.49925	–1.12960	0.00000
H	5.07199	–0.78630	0.00000

Sum of electronic and zero–point Energies: –565.831745 a.u.
N_{Im}= 2 (180*i* cm^{-1}, 80*i* cm^{-1})

6•4

	X	Y	Z
C	–2.59384	–1.53915	0.00000
C	1.32910	1.18867	0.00000
O	–1.96452	–2.56611	0.00000
N	0.57127	2.29518	0.00000
N	–2.02179	–0.28893	0.00000
N	0.84832	–0.00282	0.00000
C	–2.78382	0.84533	0.00000
C	1.74804	–1.10339	0.00000
H	–0.97180	–0.20722	0.00000
O	–2.33448	1.96849	0.00000
N	1.06411	–2.29064	0.00000
H	–3.87032	0.65600	0.00000
H	–3.69742	–1.52374	0.00000
C	3.09548	–1.04479	0.00000
H	1.01157	3.19642	0.00000
H	–0.44509	2.24813	0.00000
H	2.40195	1.38631	0.00000
H	1.57376	–3.15377	0.00000
H	0.05726	–2.33466	0.00000
H	3.67382	–1.95940	0.00000
H	3.65175	–0.12020	0.00000

Sum of electronic and zero–point Energies: –565.827803 a.u.
N_{Im}= 2 (208*i* cm^{-1}, 114*i* cm^{-1})

Table S7. Optimized Cartesian coordinates (in Å) and computed total electronic energies (including zero-point energies corrections) (in a.u.) for selected structures at ωB97XD/6-311+G(d,p) in chloroform. All the geometries were optimized with a constrained C_s symmetry.

A

	X	Y	Z
C	–2.30033	0.00077	0.00000
N	–1.14940	0.68464	0.00000
C	0.00378	0.00149	0.00000
C	–0.05049	–1.40467	0.00000
N	–2.48314	–1.31346	0.00000
C	–1.31836	–1.97120	0.00000
N	–1.09655	–3.32230	0.00000
N	0.92998	–2.37779	0.00000
C	0.26205	–3.49915	0.00000
H	–1.79829	–4.04539	0.00000
N	1.16591	0.67763	0.00000
H	0.69973	–4.48645	0.00000
H	–3.20052	0.60837	0.00000
H	2.04298	0.18698	0.00000
H	1.15558	1.68303	0.00000

Sum of electronic and zero–point Energies: –467.186252 a.u.
N_{Im}= 0

C

	X	Y	Z
C	–0.03557	–2.42645	0.00000
N	1.32504	–2.42924	0.00000
C	1.99048	–1.28701	0.00000
C	1.35344	–0.00062	0.00000
C	0.00293	–0.00301	0.00000
N	–0.67261	–1.17566	0.00000
O	–0.72734	–3.43574	0.00000
N	3.33448	–1.35383	0.00000
H	–1.68117	–1.18917	0.00000
H	–0.59269	0.90057	0.00000
H	1.91874	0.91973	0.00000
H	3.90505	–0.52743	0.00000
H	3.77760	–2.25712	0.00000

Sum of electronic and zero–point Energies: –394.832556 a.u.
N_{Im}= 0

G

	X	Y	Z
N	–2.17824	–0.86798	0.00000
C	–1.40165	0.31442	0.00000
C	–0.00787	–0.00700	0.00000
C	0.36494	–1.34187	0.00000
N	–0.42074	–2.44139	0.00000

C	–1.69901	–2.15213	0.00000
N	–2.60975	–3.14830	0.00000
O	–1.95649	1.39931	0.00000
N	1.10226	0.81324	0.00000
C	2.11302	–0.00744	0.00000
N	1.72735	–1.32717	0.00000
H	–3.17645	–0.70860	0.00000
H	2.33033	–2.13447	0.00000
H	3.15480	0.27558	0.00000
H	–2.27526	–4.09585	0.00000
H	–3.59975	–2.98153	0.00000

Sum of electronic and zero–point Energies: –542.430094 a.u.
N_{Im}= 1 (229*i* cm^{-1})

T

	X	Y	Z
N	0.00539	1.37564	0.00000
C	–1.13406	2.14257	0.00000
N	–2.29133	1.39434	0.00000
C	–2.40767	0.00367	0.00000
C	–1.13918	–0.72020	0.00000
C	–0.00364	0.00103	0.00000
O	–1.12433	3.35743	0.00000
O	–3.50930	–0.51516	0.00000
C	–1.17225	–2.21711	0.00000
H	0.97530	–0.46158	0.00000
H	0.87862	1.87929	0.00000
H	–3.15544	1.91990	0.00000
H	–0.16110	–2.62725	0.00000
H	–1.70053	–2.59375	0.87940
H	–1.70053	–2.59375	–0.87940

Sum of electronic and zero–point Energies: –454.018016 a.u.
N_{Im}= 0

U

	X	Y	Z
C	–2.45438	–1.40734	0.00000
O	–3.50430	–2.01523	0.00000
N	–2.37341	–0.03191	0.00000
C	–1.21765	0.75649	0.00000
C	0.01636	–0.00767	0.00000
N	–1.22394	–2.03012	0.00000
C	–0.03500	–1.35059	0.00000
H	–3.25753	0.45947	0.00000
O	–1.30754	1.96993	0.00000
H	0.95537	0.52400	0.00000
H	–1.23907	–3.03831	0.00000
H	0.85200	–1.97023	0.00000

Sum of electronic and zero–point Energies: –414.728657 a.u.
N_{Im}= 0

A_{imino}

	X	Y	Z
C	0.00019	0.00424	0.00000
N	1.20423	0.63291	0.00000
C	2.46168	0.00212	0.00000
C	2.28520	–1.42916	0.00000
N	–0.17439	–1.27989	0.00000
C	1.01158	–1.95502	0.00000
N	1.18422	–3.30911	0.00000
N	3.22883	–2.42631	0.00000
C	2.53269	–3.53444	0.00000
H	0.45493	–4.00498	0.00000
N	3.51584	0.72454	0.00000
H	2.94096	–4.53358	0.00000
H	–0.86254	0.66100	0.00000
H	4.33627	0.12396	0.00000
H	1.22185	1.64322	0.00000

Sum of electronic and zero–point Energies: –467.168503 a.u.
N_{Im}= 0

C_{imino}

	X	Y	Z
C	–0.10589	–1.37814	0.00000
N	1.10045	–2.03026	0.00000
C	2.37793	–1.46001	0.00000
C	2.37207	–0.00422	0.00000
C	1.20567	0.65678	0.00000
N	0.00013	–0.00304	0.00000
O	–1.17655	–1.95445	0.00000
N	3.38061	–2.25277	0.00000
H	–0.86801	0.50839	0.00000
H	1.14384	1.73682	0.00000
H	3.31187	0.52841	0.00000
H	4.24640	–1.72140	0.00000
H	1.05445	–3.03984	0.00000

Sum of electronic and zero–point Energies: –394.824945 a.u.
N_{Im}= 0

I

	X	Y	Z
N	0.79439	1.38107	0.00000
C	1.42067	0.11589	0.00000
C	2.84798	0.28376	0.00000
C	3.37621	1.56408	0.00000
N	2.70886	2.74764	0.00000
C	1.42308	2.58708	0.00000
H	0.77265	3.45431	0.00000
O	0.75821	–0.90452	0.00000
N	3.84982	–0.65761	0.00000

C	4.95277	0.04139	0.00000
N	4.72794	1.39185	0.00000
H	–0.21676	1.36383	0.00000
H	5.42323	2.12196	0.00000
H	5.95325	–0.36420	0.00000

Sum of electronic and zero–point Energies: –487.071043 a.u.
N_{Im}= 0

T_{enol}

	X	Y	Z
N	1.13099	1.98360	0.00000
C	–0.09041	1.30884	0.00000
N	–0.01976	–0.05953	0.00000
C	1.14378	–0.64826	0.00000
C	2.41615	0.00483	0.00000
C	2.33431	1.35748	0.00000
O	–1.13402	1.94141	0.00000
O	1.16894	–1.98023	0.00000
C	3.70595	–0.75859	0.00000
H	3.20766	1.99785	0.00000
H	1.08241	2.99160	0.00000
H	4.55424	–0.07217	0.00000
H	3.78321	–1.40054	0.88081
H	3.78321	–1.40054	–0.88081
H	0.25495	–2.29189	0.00000

Sum of electronic and zero–point Energies: –453.997663 a.u.
N_{Im}= 0

A•T

	X	Y	Z
C	–0.56119	0.94020	0.00000
C	3.64709	–1.27378	0.00000
N	0.10969	–0.22103	0.00000
N	2.95929	–0.07523	0.00000
C	–0.56959	–1.38313	0.00000
C	3.50336	1.18530	0.00000
C	–1.97684	–1.31006	0.00000
N	4.87972	1.19545	0.00000
N	–1.87113	1.12675	0.00000
C	5.10150	–1.17789	0.00000
C	–2.53354	–0.03843	0.00000
C	5.64266	0.05499	0.00000
N	–3.88533	–0.24976	0.00000
N	–2.95674	–2.28263	0.00000
C	–4.07342	–1.60695	0.00000
N	0.10649	–2.53655	0.00000
H	–5.06389	–2.03717	0.00000
H	0.06547	1.82770	0.00000
O	3.03223	–2.33745	0.00000
H	–0.39803	–3.40629	0.00000

H	1.12582	–2.53411	0.00000
H	1.91809	–0.12462	0.00000
O	2.83458	2.20277	0.00000
C	5.90761	–2.43945	0.00000
H	6.97595	–2.21692	0.00000
H	5.67878	–3.04663	0.87937
H	5.67878	–3.04663	–0.87937
H	6.71325	0.21811	0.00000
H	–4.60226	0.45841	0.00000
H	5.31841	2.10301	0.00000

Sum of electronic and zero–point Energies: –921.222511 a.u.
N_{Im}= 0

A•T(Hoog)

	X	Y	Z
C	–4.05090	–2.09799	0.00000
C	–2.82296	–2.79202	0.00000
N	–1.50683	–2.37379	0.00000
C	–0.80424	–3.47594	0.00000
N	–1.58284	–4.59614	0.00000
C	–2.88966	–4.17766	0.00000
N	–4.00122	–4.92084	0.00000
C	–5.09038	–4.16122	0.00000
N	–5.18033	–2.82739	0.00000
N	–4.13648	–0.76205	0.00000
O	–2.03882	1.27620	0.00000
C	–0.81101	1.28576	0.00000
N	–0.10976	0.09579	0.00000
C	1.25402	–0.05740	0.00000
O	1.80472	–1.14435	0.00000
N	1.94531	1.13201	0.00000
C	1.33226	2.36027	0.00000
C	–0.00671	2.50141	0.00000
C	–0.70344	3.82628	0.00000
H	–5.05277	–0.34603	0.00000
H	–3.31834	–0.15645	0.00000
H	–6.03942	–4.68964	0.00000
H	–1.26058	–5.55094	0.00000
H	0.27512	–3.51422	0.00000
H	–0.66417	–0.78378	0.00000
H	2.95104	1.06372	0.00000
H	2.00469	3.20906	0.00000
H	0.01854	4.64452	0.00000
H	–1.34437	3.92769	0.87934
H	–1.34437	3.92769	–0.87934

Sum of electronic and zero–point Energies: –921.222871 a.u.
N_{Im}= 0

A_{imino}•C

	X	Y	Z

C	–0.56381	0.98981	0.00000
N	–1.85506	1.16214	0.00000
C	–2.51779	–0.02581	0.00000
C	–1.97987	–1.29685	0.00000
C	–0.55079	–1.44846	0.00000
N	0.07315	–0.20233	0.00000
N	–3.87083	–0.21306	0.00000
C	–4.08336	–1.56457	0.00000
N	–2.97023	–2.25100	0.00000
N	0.17170	–2.51570	0.00000
C	3.42773	1.07372	0.00000
N	2.90651	–0.17975	0.00000
C	3.69053	–1.25685	0.00000
C	5.12396	–1.14744	0.00000
C	5.63926	0.09981	0.00000
N	4.82078	1.18158	0.00000
O	2.74343	2.09117	0.00000
N	3.10018	–2.45196	0.00000
H	0.09957	1.84877	0.00000
H	–4.57310	0.50977	0.00000
H	–5.07896	–1.98167	0.00000
H	–0.42783	–3.33570	0.00000
H	5.20020	2.11594	0.00000
H	6.70269	0.30042	0.00000
H	5.75958	–2.02059	0.00000
H	3.65837	–3.28812	0.00000
H	2.06919	–2.52540	0.00000
H	1.11407	–0.19571	0.00000

Sum of electronic and zero–point Energies: –862.026653 a.u.
N_{Im}= 0

A•C$_{imino}$

	X	Y	Z
C	–0.54785	0.92196	0.00000
N	–1.85574	1.12837	0.00000
C	–2.53435	–0.02763	0.00000
C	–1.99617	–1.30686	0.00000
C	–0.58906	–1.40171	0.00000
N	0.10608	–0.24797	0.00000
N	–3.88953	–0.21937	0.00000
C	–4.09747	–1.57366	0.00000
N	–2.99055	–2.26528	0.00000
N	0.07177	–2.56222	0.00000
C	3.48302	1.14876	0.00000
N	2.96860	–0.11709	0.00000
C	3.68743	–1.30509	0.00000
C	5.13233	–1.14414	0.00000
C	5.65798	0.09069	0.00000
N	4.86415	1.20842	0.00000
O	2.79244	2.15272	0.00000

N	3.02697	–2.40874	0.00000
H	0.09246	1.79980	0.00000
H	–4.59615	0.49900	0.00000
H	–5.09429	–1.98905	0.00000
H	–0.44972	–3.42211	0.00000
H	1.09961	–2.57440	0.00000
H	1.93091	–0.18046	0.00000
H	5.26961	2.13071	0.00000
H	6.72424	0.27467	0.00000
H	5.76711	–2.01816	0.00000
H	3.65879	–3.20317	0.00000

Sum of electronic and zero–point Energies: –862.030878 a.u.
N_{Im}= 0

A_{imino}•T_{enol}

	X	Y	Z
C	–1.49430	–0.06488	0.00000
C	2.66932	–2.54898	0.00000
N	–0.14338	–0.13222	0.00000
N	1.34832	–2.51677	0.00000
C	0.70781	0.96170	0.00000
C	0.60856	–3.66313	0.00000
C	–0.02668	2.18968	0.00000
N	1.32088	–4.85477	0.00000
N	–2.19725	1.03056	0.00000
C	3.42454	–3.77476	0.00000
C	–1.40724	2.13574	0.00000
C	2.68106	–4.90434	0.00000
N	–1.81140	3.43925	0.00000
N	0.41722	3.49058	0.00000
C	–0.67729	4.20534	0.00000
N	1.98693	0.76755	0.00000
H	–0.72299	5.28380	0.00000
H	–1.99336	–1.02767	0.00000
H	2.49136	1.64749	0.00000
H	–2.76400	3.76899	0.00000
H	0.32020	–1.06482	0.00000
H	3.11983	–5.89435	0.00000
C	4.92286	–3.76208	0.00000
H	5.31562	–4.78049	0.00000
H	5.30996	–3.24226	–0.87982
H	5.30996	–3.24226	0.87982
H	0.77866	–5.70551	0.00000
O	–0.61689	–3.67019	0.00000
O	3.34122	–1.43648	0.00000
H	2.73909	–0.57612	0.00000

Sum of electronic and zero–point Energies: –921.200581 a.u.
N_{Im}= 0

A_{imino}•T

	X	Y	Z
N	–0.78456	2.20688	0.00000
C	–0.96844	0.93430	0.00000
N	0.14060	0.08545	0.00000
C	0.08351	–1.26806	0.00000
N	–1.00183	–1.98230	0.00000
C	–2.11837	–1.20356	0.00000
C	–2.18715	0.17398	0.00000
N	–3.49259	0.60229	0.00000
C	–4.19611	–0.50022	0.00000
N	–3.41673	–1.62465	0.00000
C	3.35824	6.93196	0.00000
C	3.18645	5.44524	0.00000
C	1.82803	4.89983	0.00000
O	0.81659	5.58070	0.00000
N	1.73785	3.51027	0.00000
C	2.78215	2.63470	0.00000
O	2.64363	1.41277	0.00000
N	4.02144	3.21502	0.00000
C	4.21268	4.57732	0.00000
H	–5.27393	–0.55790	0.00000
H	1.04645	–1.76629	0.00000
H	–1.67452	2.69574	0.00000
H	–3.73504	–2.58109	0.00000
H	1.06366	0.53971	0.00000
H	0.77967	3.08470	0.00000
H	4.80920	2.58635	0.00000
H	5.24761	4.89555	0.00000
H	4.41568	7.20153	0.00000
H	2.88470	7.37630	–0.87901
H	2.88470	7.37630	0.87901

Sum of electronic and zero–point Energies: –921.207707 a.u.
N_{Im}= 0

I•A

	X	Y	Z
N	–4.07487	–0.21468	0.00000
C	–3.97277	–1.55177	0.00000
C	–2.79891	–2.29027	0.00000
C	–1.59001	–1.56455	0.00000
N	–1.67489	–0.21829	0.00000
C	–2.88526	0.36133	0.00000
H	–2.87814	1.44769	0.00000
N	–0.39190	–2.15255	0.00000
N	0.70542	1.42208	0.00000
C	1.92697	0.74181	0.00000
C	3.02296	1.66433	0.00000
C	2.74946	3.02326	0.00000
N	1.53701	3.62951	0.00000
C	0.56235	2.76970	0.00000

H	–0.46090	3.12862	0.00000
O	1.96398	–0.48543	0.00000
N	4.38068	1.43982	0.00000
C	4.90698	2.63426	0.00000
N	3.96896	3.63220	0.00000
N	–4.97307	–2.48452	0.00000
N	–3.06293	–3.64484	0.00000
H	0.46517	–1.59734	0.00000
H	–0.15277	0.83334	0.00000
H	4.14071	4.62549	0.00000
H	5.96405	2.85375	0.00000
H	–0.33939	–3.15701	0.00000
C	–4.36640	–3.71329	0.00000
H	–5.96405	–2.30157	0.00000
H	–4.94418	–4.62549	0.00000

Sum of electronic and zero–point Energies: –954.276275 a.u.
N_{Im}= 0

I•C

	X	Y	Z
N	–3.79553	0.78759	0.00000
C	–4.53470	–0.34943	0.00000
C	–3.93290	–1.55773	0.00000
C	–2.49700	–1.56394	0.00000
N	–1.79096	–0.43571	0.00000
C	–2.39891	0.77931	0.00000
O	–1.78574	1.84033	0.00000
N	–1.82247	–2.71555	0.00000
N	1.02671	–0.26542	0.00000
C	1.70154	–1.48560	0.00000
C	3.11896	–1.28172	0.00000
C	3.60130	0.01898	0.00000
N	2.89230	1.17364	0.00000
C	1.60835	0.95643	0.00000
H	0.91251	1.78901	0.00000
O	1.08123	–2.54815	0.00000
N	4.15586	–2.18748	0.00000
C	5.23180	–1.44870	0.00000
N	4.95942	–0.10637	0.00000
H	–4.24147	1.69232	0.00000
H	–5.60955	–0.22469	0.00000
H	–4.50542	–2.47329	0.00000
H	–2.31119	–3.59389	0.00000
H	–0.79943	–2.70850	0.00000
H	–0.01587	–0.31416	0.00000
H	5.62803	0.64791	0.00000
H	6.24639	–1.81793	0.00000

Sum of electronic and zero–point Energies: –881.927966 a.u.
N_{Im}= 1 (17*i* cm^{-1})

I•U

	X	Y	Z
C	–2.69446	–0.02636	0.00000
O	–2.09275	1.04275	0.00000
N	0.72334	1.29911	0.00000
C	1.38939	0.06974	0.00000
C	2.80803	0.26228	0.00000
C	3.30335	1.55737	0.00000
N	2.60373	2.71868	0.00000
C	1.32068	2.51692	0.00000
H	0.64613	3.36546	0.00000
O	0.76131	–0.98551	0.00000
N	3.83481	–0.65320	0.00000
C	4.91811	0.07473	0.00000
N	4.65899	1.41976	0.00000
H	–0.30498	1.25141	0.00000
H	5.33526	2.16733	0.00000
H	5.92878	–0.30482	0.00000
N	–2.07336	–1.24169	0.00000
C	–2.69692	–2.49535	0.00000
C	–4.15000	–2.44161	0.00000
N	–4.06582	–0.07553	0.00000
C	–4.77086	–1.25170	0.00000
H	–1.04181	–1.22174	0.00000
O	–2.02985	–3.51166	0.00000
H	–4.70195	–3.36906	0.00000
H	–4.54373	0.81233	0.00000
H	–5.84748	–1.14748	0.00000

Sum of electronic and zero–point Energies: –901.816772 a.u.
N_{Im}= 0

G•U

	X	Y	Z
C	–2.68788	0.01885	0.00000
O	–2.08826	1.09103	0.00000
N	0.71720	1.28048	0.00000
C	1.40730	0.06493	0.00000
C	2.81774	0.27112	0.00000
C	3.28881	1.57694	0.00000
N	2.58483	2.72817	0.00000
C	1.28778	2.52248	0.00000
N	0.43677	3.56985	0.00000
O	0.77946	–0.99341	0.00000
N	3.86415	–0.62947	0.00000
C	4.93210	0.11432	0.00000
N	4.64638	1.45998	0.00000
H	–0.30803	1.20547	0.00000
H	5.30873	2.21938	0.00000
H	5.95038	–0.24440	0.00000
N	–2.06492	–1.19470	0.00000

C	–2.68992	–2.44897	0.00000
C	–4.14321	–2.39540	0.00000
N	–4.05823	–0.03003	0.00000
C	–4.76433	–1.20600	0.00000
H	–1.03143	–1.18027	0.00000
O	–2.02357	–3.46515	0.00000
H	–4.69465	–3.32320	0.00000
H	–4.53522	0.85817	0.00000
H	–5.84093	–1.10098	0.00000
H	0.81744	4.49940	0.00000
H	–0.56033	3.44267	0.00000

Sum of electronic and zero–point Energies: –957.177318 a.u.
N_{Im}= 1 (205*i* cm^{-1})

Table S8. Gas-phase optimized structures, at C_s vs. C_1 symmetry, at ωB97X-D/6-311+G(d,p) for structures with a nonplanar minimum.

C

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–0.08337	–1.41602	0.00000	C	–0.11186	–1.40314	–0.01094
N	1.10497	–2.09173	0.00000	N	1.06619	–2.08411	–0.14331
C	2.24040	–1.43520	0.00000	C	2.20441	–1.43470	–0.19577
C	2.34044	0.00039	0.00000	C	2.31802	–0.00187	–0.12516
C	1.17035	0.67501	0.00000	C	1.15810	0.67800	0.00393
N	0.00015	–0.00024	0.00000	N	–0.01492	0.01001	0.05944
O	–1.18123	–1.92722	0.00000	O	–1.21112	–1.90781	0.04818
N	3.37700	–2.16944	0.00000	N	3.33159	–2.17454	–0.31507
H	–0.88476	0.48233	0.00000	H	–0.89235	0.49659	0.15594
H	1.11149	1.75661	0.00000	H	1.10987	1.75823	0.06795
H	3.29074	0.51418	0.00000	H	3.27056	0.50581	–0.16901
H	4.28524	–1.74454	0.00000	H	4.23361	–1.75147	–0.42959
H	3.29292	–3.17170	0.00000	H	3.23344	–3.17151	–0.40573
Sum of electronic and ZPE corrections:							
	–394.816334				–394.816133		
Sum of electronic and thermal free energy:							
	–394.846744				–394.847574		
N_{Im} in C_s optimized structure = 1 (55i cm^{-1})							

G

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–3.56382	–0.99855	0.00000	N	–3.56784	–0.99517	0.03375
C	–2.56051	0.01921	0.00000	C	–2.56440	0.02094	–0.00093
C	–1.25907	–0.58860	0.00000	C	–1.26308	–0.59013	–0.01418
C	–1.17217	–1.97063	0.00000	C	–1.17755	–1.97127	0.01333
N	–2.16501	–2.89255	0.00000	N	–2.17432	–2.89087	0.03254
C	–3.35126	–2.34953	0.00000	C	–3.35652	–2.34522	0.04965
N	–4.44929	–3.14876	0.00000	N	–4.46937	–3.14055	0.13361
O	–2.89791	1.17935	0.00000	O	–2.89719	1.18194	–0.00724
N	–0.00592	–0.01663	0.00000	N	–0.00992	–0.02034	–0.03807
C	0.81355	–1.02412	0.00000	C	0.80846	–1.02930	–0.02666
N	0.16382	–2.24050	0.00000	N	0.15776	–2.24395	0.00406
H	–4.50508	–0.63227	0.00000	H	–4.50772	–0.63309	0.11206
H	–5.38475	–2.78878	0.00000	H	–5.32504	–2.80750	–0.27964
H	–4.30139	–4.14178	0.00000	H	–4.27988	–4.11935	–0.01213
H	0.57650	–3.15824	0.00000	H	0.56941	–3.16210	0.01909
H	1.89137	–0.95830	0.00000	H	1.88627	–0.96470	–0.03924
Sum of electronic and ZPE corrections:							
	–542.410714				–542.410490		
Sum of electronic and thermal free energy:							
	–542.443568				–542.443493		
N_{Im} in C_s optimized structure = 1 (327i cm^{-1})							

8-oxoG

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	3.64565	0.33262	0.00000	C	1.29979	1.58369	–0.15540
C	2.27028	0.00227	0.00000	C	1.20078	0.17116	–0.15003
N	1.12553	0.79484	0.00000	N	2.17141	–0.82544	–0.16130
C	–0.00311	0.00479	0.00000	C	1.57929	–2.07034	–0.16469
N	0.49626	–1.30698	0.00000	N	0.20328	–1.79517	–0.15550
C	1.86565	–1.30880	0.00000	C	–0.02440	–0.44483	–0.14828
N	2.64850	–2.40657	0.00000	N	–1.23667	0.14847	–0.13056
C	3.92817	–2.13264	0.00000	C	–1.17659	1.45323	–0.13872
N	4.42286	–0.86090	0.00000	N	–0.00520	2.15149	–0.14898
N	4.82230	–3.15250	0.00000	N	–2.33436	2.17999	–0.18529
O	–1.16440	0.33844	0.00000	O	2.10157	–3.15952	–0.17291
H	1.09606	1.79928	0.00000	H	3.16688	–0.68771	–0.16754
H	5.41952	–0.69658	0.00000	H	–0.01449	3.15952	–0.21707
O	4.19159	1.41961	0.00000	O	2.28303	2.29891	–0.16924
H	–0.09921	–2.11750	0.00000	H	–0.49758	–2.51655	–0.15712
H	5.81436	–3.00805	0.00000	H	–2.34185	3.10273	0.21707
H	4.45890	–4.08869	0.00000	H	–3.16688	1.63504	–0.02719
Sum of electronic and ZPE corrections:							
		–617.662717				–617.662312	
Sum of electronic and thermal free energy:							
		–617.697231				–617.696949	
N_{Im} in C_s optimized structure = 1 (312i cm^{-1})							

yC

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.07353	1.16765	0.00000	C	0.11044	1.22084	–0.08277
N	0.01442	–0.12665	0.00000	N	0.02928	–0.06917	–0.10907
C	1.18008	–0.87577	0.00000	C	1.18484	–0.83886	–0.06122
O	1.15922	–2.08853	0.00000	O	1.14107	–2.05010	–0.05165
C	2.47306	–0.12903	0.00000	C	2.48776	–0.11233	–0.03595
C	2.46455	1.26442	0.00000	C	2.50036	1.28125	–0.01926
N	1.22818	1.90075	0.00000	N	1.27410	1.93660	–0.04619
N	–1.08539	1.87548	0.00000	N	–1.04093	1.96488	–0.05061
C	3.65692	1.98954	0.00000	C	3.70349	1.98757	0.02025
H	1.19713	2.90663	0.00000	H	1.24607	2.93048	0.11252
H	–1.93827	1.34436	0.00000	H	3.70110	3.07266	0.03157
H	–1.12380	2.87741	0.00000	C	4.89454	1.28421	0.04250
H	3.63840	3.07466	0.00000	H	5.83197	1.82779	0.07411
C	4.85930	1.30480	0.00000	C	4.89889	–0.11250	0.02222
H	5.78852	1.86326	0.00000	H	5.83857	–0.65130	0.03826
C	4.88484	–0.09151	0.00000	C	3.70047	–0.80165	–0.01603
H	5.83284	–0.61581	0.00000	H	3.66493	–1.88466	–0.02851
C	3.69618	–0.79909	0.00000	H	–1.03945	2.87001	–0.49279
H	3.67644	–1.88260	0.00000	H	–1.86889	1.41265	–0.21229
Sum of electronic and ZPE corrections:							
		–548.390209				–548.389928	

Sum of electronic and thermal free energy:							
	–548.424540				–548.424327		
N_{Im} in C_s optimized structure = 1 (324*i* cm^{-1})							

IsoG

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.94177	0.84402	0.00000	C	0.97853	–0.06163	0.79973
C	–0.22768	0.10623	0.00000	C	–0.21849	0.04822	0.11831
C	–0.09065	–1.29263	0.00000	C	–0.15005	0.01381	–1.28585
N	0.99606	–2.03288	0.00000	N	0.89378	–0.10737	–2.07519
C	2.16348	–1.34114	0.00000	C	2.08773	–0.21709	–1.43851
N	2.07423	0.10902	0.00000	N	2.06892	–0.18436	0.01322
N	0.98213	2.18817	0.00000	N	1.08367	–0.07611	2.14350
O	3.28516	–1.79974	0.00000	O	3.17934	–0.34058	–1.94968
N	–1.55719	0.49711	0.00000	N	–1.52005	0.19875	0.57021
C	–2.20903	–0.62264	0.00000	C	–2.22131	0.25145	–0.51784
N	–1.38936	–1.73555	0.00000	N	–1.46136	0.14587	–1.66765
H	–3.28516	–0.71656	0.00000	H	–3.29452	0.36644	–0.56167
H	–1.66931	–2.70231	0.00000	H	–1.78622	0.16372	–2.62009
H	1.84408	2.70231	0.00000	H	1.97155	0.03607	2.60004
H	0.11063	2.69051	0.00000	H	0.25001	0.11712	2.67382
H	2.98067	0.55373	0.00000	H	2.98809	–0.29323	0.41669
Sum of electronic and ZPE corrections:							
	–542.403977				–542.403571		
Sum of electronic and thermal free energy:							
	–542.436885				–542.436921		
N_{Im} in C_s optimized structure = 1 (132*i* cm^{-1})							

IsoC

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.03440	1.24120	0.00000	C	–0.04777	0.00513	–1.22723
N	0.03459	–0.15460	0.00000	N	0.06207	0.02023	0.16829
C	1.15116	–0.80331	0.00000	C	1.22232	–0.04475	0.72459
N	1.13725	–2.16332	0.00000	N	1.32853	–0.11148	2.09386
N	2.38884	–0.20762	0.00000	N	2.40861	–0.09597	0.03670
C	2.46962	1.17090	0.00000	C	2.38394	–0.08598	–1.34325
C	1.35213	1.90500	0.00000	C	1.21412	–0.02268	–1.98904
O	–1.00057	1.87491	0.00000	O	–1.12939	0.02439	–1.77501
H	3.22893	–0.75969	0.00000	H	3.26779	–0.28375	0.52494
H	3.47042	1.58319	0.00000	H	3.34861	–0.12659	–1.83249
H	1.38627	2.98513	0.00000	H	1.16560	–0.00505	–3.06851
H	1.96610	–2.72725	0.00000	H	2.11530	0.34601	2.52711
H	0.23532	–2.60584	0.00000	H	0.44696	0.05236	2.55596
Sum of electronic and ZPE corrections:							
	–394.800066				–394.799944		
Sum of electronic and thermal free energy:							
	–394.830807				–394.830757		
N_{Im} in C_s optimized structure = 1 (354*i* cm^{-1})							

K

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.16426	1.22179	0.00000	C	–1.12743	0.09860	0.46404
N	0.08849	–0.11483	0.00000	N	0.06633	0.02265	–0.13614
C	1.24398	–0.77620	0.00000	C	0.06523	0.02357	–1.46681
N	1.16608	–2.13207	0.00000	N	1.28035	–0.09169	–2.07707
C	2.48070	–0.10416	0.00000	C	–1.12917	0.10417	–2.20449
C	2.41577	1.27191	0.00000	C	–2.28910	0.17374	–1.46396
N	1.27713	1.96565	0.00000	N	–2.32310	0.17086	–0.13108
N	–1.01532	1.89185	0.00000	N	–1.11874	0.13207	1.82545
H	1.98878	–2.70462	0.00000	H	1.36595	0.14919	–3.04847
H	0.25830	–2.56185	0.00000	H	2.08982	0.04080	–1.49407
H	–1.00633	2.89485	0.00000	H	–1.99676	–0.00289	2.29487
H	–1.87703	1.37905	0.00000	H	–0.26863	–0.12464	2.29494
H	3.32888	1.86159	0.00000	H	–3.25327	0.23333	–1.96209
H	3.42424	–0.63336	0.00000	H	–1.13932	0.10041	–3.28626
Sum of electronic and ZPE corrections:							
	–374.938012				–374.937013		
Sum of electronic and thermal free energy:							
	–374.968212				–374.967685		
N_{Im} in C_s optimized structure = 2 (226*i* cm^{-1}, 198*i* cm^{-1})							

Pi

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.92322	1.20747	0.00000	C	–1.39820	–0.14747	0.59156
C	–0.28338	0.40726	0.00000	C	0.04079	0.00920	0.50067
C	–0.26223	–0.97157	0.00000	C	0.69936	0.07878	–0.70985
N	0.93593	–1.65856	0.00000	N	0.00628	–0.00227	–1.90179
C	2.14755	–1.00550	0.00000	C	–1.36001	–0.15547	–1.93789
N	2.05538	0.38882	0.00000	N	–1.96739	–0.21906	–0.68107
O	1.00309	2.41571	0.00000	O	–2.07294	–0.21339	1.59575
O	3.21205	–1.57717	0.00000	O	–1.99699	–0.23023	–2.96191
N	–1.58979	0.77948	0.00000	N	0.99081	0.12371	1.46682
N	–2.38944	–0.27642	0.00000	N	2.19848	0.25630	0.94108
C	–1.60967	–1.35804	0.00000	C	2.05341	0.23427	–0.38323
H	2.94716	0.86461	0.00000	H	–2.97178	–0.32926	–0.70961
H	0.97756	–2.66435	0.00000	H	0.46878	0.04727	–2.79454
C	–2.12843	2.12753	0.00000	C	0.81383	0.08481	2.90803
H	–3.21205	2.03443	0.00000	H	2.91282	0.33113	–1.02765
H	–1.79250	2.66435	0.88711	H	1.27458	0.96926	3.34698
H	–1.79250	2.66435	–0.88711	H	–0.25346	0.06912	3.11944
H	–2.04692	–2.34383	0.00000	H	1.28594	–0.81234	3.31004
Sum of electronic and ZPE corrections:							
	–601.567341				–601.567229		
Sum of electronic and thermal free energy:							
	–601.601784				–601.603663		
N_{Im} in C_s optimized structure = 1 (93*i* cm^{-1})							

G*

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–3.61517	–0.97236	0.00000	N	–3.54717	–0.01834	1.20768
C	–2.59802	–0.12994	0.00000	C	–2.58704	–0.01241	0.30045
C	–1.28207	–0.60294	0.00000	C	–1.24333	–0.01092	0.68748
C	–1.17124	–1.99425	0.00000	C	–1.04280	–0.02243	2.06857
N	–2.15987	–2.88417	0.00000	N	–1.97264	–0.03094	3.01999
C	–3.35766	–2.29961	0.00000	C	–3.20476	–0.02161	2.51456
N	–4.44635	–3.10988	0.00000	N	–4.24294	0.01547	3.39774
O	–2.85946	1.17370	0.00000	O	–2.93244	–0.01007	–0.98325
N	–0.03534	–0.00308	0.00000	N	–0.03822	–0.00698	0.00837
C	0.79505	–0.99926	0.00000	C	0.85479	–0.01539	0.94897
N	0.17461	–2.23339	0.00000	N	0.31563	–0.02578	2.22036
H	–5.36377	–2.70559	0.00000	H	–5.15872	–0.19839	3.04448
H	–4.31922	–4.10469	0.00000	H	–4.03706	–0.19522	4.35848
H	0.61220	–3.13916	0.00000	H	0.81097	–0.02963	3.09591
H	1.87190	–0.91276	0.00000	H	1.92379	–0.01464	0.79297
H	–3.81891	1.26598	0.00000	H	–3.89586	–0.00640	–1.01351
Sum of electronic and ZPE corrections:							
	–542.408543				–542.408034		
Sum of electronic and thermal free energy:							
	–542.441172				–542.440881		
N_{Im} in C_s optimized structure = 1 (219i cm^{-1})							

6-thioG

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.32871	1.09109	0.00000	C	0.39188	0.01074	–1.07400
C	–0.77709	0.19945	0.00000	C	–0.75948	0.00080	–0.23970
C	–0.53172	–1.16870	0.00000	C	–0.58619	–0.00067	1.13870
N	0.65545	–1.81148	0.00000	N	0.56810	–0.01255	1.84138
C	1.66828	–0.98590	0.00000	C	1.61973	0.00143	1.06986
N	1.53421	0.37486	0.00000	N	1.55736	0.01604	–0.29508
S	0.35580	2.74305	0.00000	S	0.50115	0.02387	–2.72164
N	2.93143	–1.47973	0.00000	N	2.86799	0.04959	1.62589
N	–2.13237	0.44863	0.00000	N	–2.09920	0.00044	–0.55919
C	–2.68321	–0.72577	0.00000	C	–2.71085	–0.00124	0.58526
N	–1.76060	–1.75311	0.00000	N	–1.84362	–0.00236	1.65887
H	3.04067	–2.47781	0.00000	H	2.88296	–0.11654	2.61921
H	3.74527	–0.89416	0.00000	H	3.64230	–0.33728	1.11204
H	–3.74527	–0.92134	0.00000	H	–3.78169	–0.00166	0.72489
H	2.35630	0.96349	0.00000	H	2.41076	0.07765	–0.83412
H	–1.94173	–2.74305	0.00000	H	–2.07622	–0.00317	2.63807
Sum of electronic and ZPE corrections:							
	–865.373500				–865.373127		
Sum of electronic and thermal free energy:							
	–865.407221				–865.407000		
N_{Im} in C_s optimized structure = 1 (302i cm^{-1})							

2-aminoA

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–0.64543	1.04264	0.00000	C	1.14372	0.04033	0.44729
N	0.08693	–0.09114	0.00000	N	–0.12207	–0.01516	–0.01419
C	–0.55161	–1.25809	0.00000	C	–0.31777	–0.03950	–1.33011
C	–1.95855	–1.27249	0.00000	C	0.79461	–0.00502	–2.19058
N	–1.97631	1.16217	0.00000	N	2.27572	0.06452	–0.25993
C	–2.57271	–0.02866	0.00000	C	2.03411	0.04333	–1.56966
N	–3.91424	–0.30845	0.00000	N	2.93482	0.06283	–2.60212
N	–2.88833	–2.29621	0.00000	N	0.91852	–0.01411	–3.56781
C	–4.03428	–1.68280	0.00000	C	2.20195	0.02756	–3.77002
N	0.16849	–2.39863	0.00000	N	–1.57936	–0.10828	–1.80344
H	–5.00127	–2.16394	0.00000	H	2.68261	0.03540	–4.73722
N	0.07161	2.19732	0.00000	N	1.26778	0.10749	1.80704
H	–0.29912	–3.28743	0.00000	H	–1.74412	–0.06493	–2.79339
H	1.17133	–2.34682	0.00000	H	–2.34665	–0.06251	–1.15692
H	–4.65784	0.36888	0.00000	H	3.93581	0.10187	–2.51095
H	–0.41069	3.07636	0.00000	H	2.17745	–0.08461	2.18896
H	1.07310	2.15361	0.00000	H	0.46120	–0.15071	2.34800
Sum of electronic and ZPE corrections:							
	–522.535242				–522.534740		
Sum of electronic and thermal free energy:							
	–522.568807				–522.568372		
N_{Im} in C_s optimized structure = 1 (250i cm^{-1})							

G•U

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	5.33054	–1.34302	0.00000	C	–2.67394	0.00570	–0.00702
O	4.45425	–2.20296	0.00000	O	–2.08412	1.08225	–0.00709
N	1.71245	–1.58046	0.00000	N	0.71865	1.29232	0.05980
C	1.41350	–0.20797	0.00000	C	1.40209	0.06513	0.03190
C	–0.00088	0.00339	0.00000	C	2.81725	0.27290	0.00958
C	–0.82680	–1.11197	0.00000	C	3.28452	1.57929	0.00695
N	–0.49232	–2.42129	0.00000	N	2.58373	2.73514	0.02258
C	0.80475	–2.59806	0.00000	C	1.29271	2.52847	0.05394
N	1.31741	–3.85289	0.00000	N	0.43653	3.58580	0.11950
O	2.32667	0.60667	0.00000	O	0.76537	–0.97950	0.02863
N	–0.74231	1.16566	0.00000	N	3.86307	–0.62439	–0.01691
C	–1.97670	0.76499	0.00000	C	4.92835	0.11694	–0.03399
N	–2.09428	–0.61010	0.00000	N	4.64284	1.46683	–0.02137
H	2.71372	–1.80559	0.00000	H	–0.30512	1.21769	0.07159
H	–2.94002	–1.15515	0.00000	H	5.29445	2.23350	–0.02797
H	–2.84563	1.40624	0.00000	H	5.94553	–0.24518	–0.05568
N	5.09382	–0.00339	0.00000	N	–2.05938	–1.20796	0.00728
C	6.06736	1.01621	0.00000	C	–2.69535	–2.46592	0.00913
C	7.44552	0.52689	0.00000	C	–4.15606	–2.39715	–0.00656
N	6.65933	–1.70402	0.00000	N	–4.05029	–0.03404	–0.02202

C	7.68676	–0.78960	0.00000	C	–4.76846	–1.20706	–0.02096
H	4.10043	0.29262	0.00000	H	–1.02328	–1.20248	0.01748
O	5.74496	2.17811	0.00000	O	–2.04988	–3.48441	0.02259
H	8.24217	1.25515	0.00000	H	–4.70747	–3.32503	–0.00587
H	6.83941	–2.69445	0.00000	H	–4.50966	0.86169	–0.02880
H	8.68433	–1.20973	0.00000	H	–5.84492	–1.09417	–0.03259
H	0.67720	–4.62551	0.00000	H	0.83631	4.48811	–0.07249
H	2.30859	–4.01574	0.00000	H	–0.53531	3.44677	–0.10263
Sum of electronic and ZPE corrections:							
	–957.152734				–957.152109		
Sum of electronic and thermal free energy:							
	–957.198314				–957.197855		
N_{Im} in C_s optimized structure = 1 (220*i* cm^{-1})							

8-oxoG•A

	C_s			C_1			
	X	Y	Z		X	Y	Z
C	–2.67185	1.63132	0.00000	C	–2.64793	1.65935	0.03546
C	–2.75364	0.22719	0.00000	C	–2.73765	0.25388	0.04088
N	–1.77456	–0.75452	0.00000	N	–1.76395	–0.73120	0.03242
C	–2.35874	–1.99245	0.00000	C	–2.35410	–1.96733	0.02892
N	–3.74643	–1.73603	0.00000	N	–3.74020	–1.70441	0.03574
C	–3.98427	–0.39259	0.00000	C	–3.97055	–0.35959	0.04158
N	–5.19581	0.19807	0.00000	N	–5.17918	0.24035	0.05909
C	–5.13978	1.50467	0.00000	C	–5.11475	1.54384	0.05074
N	–3.96693	2.20338	0.00000	N	–3.93933	2.23645	0.03963
N	1.18292	1.85876	0.00000	N	1.21055	1.86148	0.00185
C	1.77561	0.66019	0.00000	C	1.79402	0.65839	–0.00047
N	1.03291	–0.45957	0.00000	N	1.04297	–0.45576	0.00984
C	3.17678	0.50499	0.00000	C	3.19380	0.49264	–0.01326
N	–6.29376	2.21908	0.00000	N	–6.26914	2.27971	0.00185
O	–1.83606	–3.08558	0.00000	O	–1.83560	–3.06211	0.02225
H	–0.74779	–0.60146	0.00000	H	–0.73578	–0.58345	0.02521
C	1.63610	–1.66021	0.00000	C	1.63725	–1.66100	0.00715
C	3.65582	–0.79632	0.00000	C	3.66327	–0.81214	–0.01429
H	–3.96852	3.21338	0.00000	H	–3.94305	3.24420	–0.03174
H	–6.31546	3.22129	0.00000	H	1.79545	2.67902	–0.00804
H	–7.15686	1.70585	0.00000	N	2.93157	–1.93155	–0.00444
H	1.76173	2.68067	0.00000	H	0.95453	–2.50719	0.01534
N	2.93254	–1.92121	0.00000	N	4.23298	1.40100	–0.02575
H	0.95974	–2.51152	0.00000	N	5.02835	–0.68870	–0.02776
N	4.20944	1.42090	0.00000	C	5.30218	0.65781	–0.03408
N	5.02006	–0.66288	0.00000	H	6.31712	1.02745	–0.04491
C	5.28412	0.68557	0.00000	H	0.19734	1.96867	0.00873
H	6.29636	1.06269	0.00000	O	–1.66014	2.38817	0.02232
H	0.16871	1.95845	0.00000	H	5.68872	–1.44799	–0.03239
O	–1.68938	2.36846	0.00000	H	–4.43706	–2.42961	0.03439
H	5.68586	–1.41741	0.00000	H	–6.27300	3.19084	0.43079
H	–4.43968	–2.46463	0.00000	H	–7.10227	1.73459	0.15785
Sum of electronic and ZPE corrections:							

		–1084.862524				–1084.862267	
Sum of electronic and thermal free energy:							
		–1084.910640				–1084.910541	
N_{Im} in C_s optimized structure = 1 (329*i* cm^{-1})							

Reverse G•U

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–0.00710	0.06116	0.00000	C	–2.70200	0.05745	–0.00462
O	0.96152	0.81846	0.00000	O	–2.06369	1.10808	0.00020
N	3.62121	–0.01900	0.00000	N	0.71862	1.27579	0.06861
C	3.82531	–1.40684	0.00000	C	1.40046	0.04985	0.04181
C	5.22124	–1.71618	0.00000	C	2.81548	0.25510	0.01231
C	6.12183	–0.65982	0.00000	C	3.28352	1.56161	0.00214
N	5.87853	0.66903	0.00000	N	2.58438	2.71789	0.01762
C	4.59586	0.93419	0.00000	C	1.29256	2.51163	0.05575
N	4.16825	2.21982	0.00000	N	0.43629	3.56706	0.11934
O	2.85720	–2.15746	0.00000	O	0.76177	–0.99515	0.04448
N	5.88134	–2.92673	0.00000	N	3.86088	–0.64300	–0.01643
C	7.14028	–2.61157	0.00000	C	4.92640	0.09769	–0.04197
N	7.35193	–1.24779	0.00000	N	4.64175	1.44783	–0.03293
H	2.63610	0.27684	0.00000	H	–0.30758	1.20346	0.07916
H	8.23304	–0.76203	0.00000	H	5.29365	2.21413	–0.04597
H	7.96323	–3.31087	0.00000	H	5.94329	–0.26503	–0.06771
N	0.16312	–1.31019	0.00000	N	–2.05826	–1.16517	0.01767
C	–0.84069	–2.26166	0.00000	C	–2.66062	–2.41014	0.01658
N	–2.12387	–1.71747	0.00000	N	–4.05302	–2.35502	–0.01036
C	–1.38091	0.52500	0.00000	C	–4.15083	0.00532	–0.03297
C	–2.37705	–0.37727	0.00000	C	–4.76351	–1.19090	–0.03432
H	1.13420	–1.67727	0.00000	H	–1.02061	–1.16425	0.03375
O	–0.65324	–3.45040	0.00000	O	–2.06490	–3.45565	0.03661
H	–2.87146	–2.39275	0.00000	H	–4.51359	–3.25099	–0.01131
H	–1.56662	1.58768	0.00000	H	–4.70016	0.93359	–0.05069
H	–3.42256	–0.09534	0.00000	H	–5.84098	–1.29697	–0.05388
H	4.85797	2.94852	0.00000	H	0.83032	4.47208	–0.07004
H	3.18933	2.44717	0.00000	H	–0.54146	3.42497	–0.07382
Sum of electronic and ZPE corrections:							
		–957.155034				–957.154502	
Sum of electronic and thermal free energy:							
		–957.200472				–957.200180	
N_{Im} in C_s optimized structure = 1 (192*i* cm^{-1})							

K•Pi

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.14595	1.22543	0.00000	C	–1.31706	–2.95092	–0.19785
N	0.07169	–0.12203	0.00000	N	–1.78878	–1.69671	–0.04513
C	1.23426	–0.79231	0.00000	C	–3.11377	–1.56122	0.11272
N	1.18223	–2.13988	0.00000	N	–3.60047	–0.31250	0.28779
C	2.46715	–0.10930	0.00000	C	–3.96256	–2.68545	0.11700

C	2.40377	1.26408	0.00000	C	–3.35616	–3.90856	–0.04828
N	1.26701	1.95895	0.00000	N	–2.04356	–4.07542	–0.20608
C	–3.64703	–0.71767	0.00000	C	1.35757	0.34836	0.03434
C	–4.85875	–1.50508	0.00000	C	2.14763	1.56155	0.03289
C	–4.84348	–2.88275	0.00000	C	1.56927	2.80982	–0.05754
N	–3.64215	–3.56039	0.00000	N	0.19839	2.93811	–0.14098
C	–2.44087	–2.89537	0.00000	C	–0.62792	1.84284	–0.12990
N	–2.50923	–1.51118	0.00000	N	–0.00109	0.61018	–0.04524
O	–3.59262	0.49995	0.00000	O	1.79297	–0.78935	0.09365
O	–1.38055	–3.49519	0.00000	O	–1.83965	1.95402	–0.19125
N	–6.16404	–1.12815	0.00000	N	3.49190	1.76016	0.08843
N	–6.96658	–2.18224	0.00000	N	3.78894	3.04985	0.04638
C	–6.19133	–3.26688	0.00000	C	2.63863	3.71555	–0.04611
N	–1.01632	1.90949	0.00000	N	0.01487	–3.09285	–0.37999
H	–1.58793	–1.01716	0.00000	H	–0.64081	–0.21697	–0.04668
H	2.03445	–2.66870	0.00000	H	–4.59517	–0.17736	0.28063
H	0.29554	–2.63497	0.00000	H	–3.00950	0.49605	0.11576
H	–0.95870	2.91148	0.00000	H	0.36671	–4.03374	–0.38059
H	–1.91605	1.44511	0.00000	H	0.65020	–2.32388	–0.20270
H	–3.58942	–4.56581	0.00000	H	–0.25635	3.83440	–0.20061
C	–6.70144	0.22056	0.00000	C	4.54161	0.76702	0.23597
H	–7.78510	0.12791	0.00000	H	5.32596	0.97611	–0.49016
H	–6.36529	0.75680	0.88728	H	4.95356	0.81312	1.24514
H	–6.36529	0.75680	–0.88728	H	4.10882	–0.21538	0.05962
H	3.31765	1.85305	0.00000	H	–3.95240	–4.81761	–0.05514
H	3.40930	–0.64080	0.00000	H	–5.03227	–2.58757	0.24457
H	–6.63218	–4.25100	0.00000	H	2.63452	4.79256	–0.10201
Sum of electronic and ZPE corrections:							
	–976.532423				–976.531906		
Sum of electronic and thermal free energy:							
	–976.577428				–976.580006		
N_{Im} in C_s optimized structure = 2 (134*i* cm^{-1}, 20*i* cm^{-1})							

Reverse G•C

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–1.03272	–0.84626	0.00000	C	–0.26840	1.85926	0.39570
C	2.89211	0.91383	0.00000	C	2.76991	1.06838	–0.46518
N	–0.97616	0.51685	0.00000	N	–0.12469	1.40701	–0.88897
N	3.10552	–0.43231	0.00000	N	2.40131	0.54106	0.73078
C	–2.08899	1.39983	0.00000	C	–0.44393	0.11393	–1.36848
C	4.33415	–0.90913	0.00000	C	2.13553	–0.74686	0.82442
C	–3.31550	0.64638	0.00000	C	–1.11971	–0.62899	–0.34119
C	5.50267	–0.07455	0.00000	C	2.28952	–1.66924	–0.25967
N	–2.15132	–1.53384	0.00000	N	–0.90994	1.19003	1.32057
N	4.02448	1.74243	0.00000	N	2.99829	0.17425	–1.51755
C	–3.24215	–0.73573	0.00000	C	–1.32555	–0.01928	0.88606
C	5.28697	1.25902	0.00000	C	2.71735	–1.14746	–1.42874
N	–4.54049	–1.15917	0.00000	N	–1.98083	–0.95263	1.63749
N	–4.62841	1.06947	0.00000	N	–1.62290	–1.91274	–0.34444

C	–5.32659	–0.02555	0.00000	C	–2.13168	–2.06873	0.84104
H	–6.40500	–0.08464	0.00000	H	–2.63232	–2.95649	1.19876
N	0.14607	–1.51314	0.00000	N	0.28230	3.07771	0.65929
O	1.79077	1.43233	0.00000	O	2.86147	2.27143	–0.68715
N	4.48049	–2.24864	0.00000	N	1.69353	–1.19454	2.02388
H	6.08789	1.98752	0.00000	H	2.83436	–1.73118	–2.33173
H	–4.84304	–2.11829	0.00000	H	–2.30942	–0.81931	2.57932
H	6.50167	–0.48499	0.00000	H	2.03017	–2.71345	–0.16950
H	3.83669	2.73377	0.00000	H	3.21637	0.59387	–2.40818
H	0.08801	–2.51485	0.00000	H	0.26411	3.29232	1.64483
H	1.05084	–1.05933	0.00000	H	1.20409	3.20815	0.24433
H	–0.05925	0.96470	0.00000	H	0.37821	1.99101	–1.54411
O	–1.91147	2.59783	0.00000	O	–0.13002	–0.20729	–2.49635
H	5.38547	–2.68190	0.00000	H	1.24557	–2.09281	2.07807
H	3.65740	–2.82626	0.00000	H	1.40450	–0.48677	2.68060
Sum of electronic and ZPE corrections:							
		–937.249539				–937.254939	
Sum of electronic and thermal free energy:							
		–937.294481				–937.299053	
N_{Im} in C_s optimized structure = 2 (74*i* cm^{-1}, 4*i* cm^{-1})							

G•A$_{imino}$

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–2.60005	1.05099	0.00000	C	2.00248	0.49062	1.90689
C	–2.88838	–0.34686	0.00000	C	0.87937	0.23160	2.75046
N	–2.04012	–1.43220	0.00000	N	–0.46593	0.20158	2.45837
C	–2.83085	–2.46354	0.00000	C	–1.03904	–0.07404	3.59225
N	–4.16339	–2.11241	0.00000	N	–0.13634	–0.22684	4.62147
C	–4.21259	–0.75039	0.00000	C	1.10342	–0.03142	4.09037
N	–5.32889	0.01074	0.00000	N	2.28028	–0.09872	4.75300
C	–5.06808	1.29055	0.00000	C	3.30649	0.14317	3.98558
N	–3.79623	1.80346	0.00000	N	3.20300	0.42395	2.64813
N	1.87464	2.67259	0.00000	N	1.62222	0.27730	–2.74812
C	2.11962	1.42197	0.00000	C	0.38482	0.17038	–2.46296
N	1.12656	0.40858	0.00000	N	–0.15382	0.31243	–1.15787
C	3.43053	0.80483	0.00000	C	–0.68921	–0.11246	–3.39342
N	–6.08956	2.17948	0.00000	N	4.56055	0.16809	4.52066
C	1.35165	–0.92943	0.00000	C	–1.46163	0.19407	–0.81679
C	3.52199	–0.57151	0.00000	C	–1.98080	–0.20072	–2.91744
H	–3.64956	2.80333	0.00000	H	4.03036	0.65032	2.11344
H	–5.94971	3.17249	0.00000	H	5.35290	–0.02430	3.93095
H	–7.02495	1.81361	0.00000	H	4.62112	–0.17861	5.46426
N	2.51802	–1.49665	0.00000	N	–2.43344	–0.05980	–1.63706
H	0.44961	–1.53295	0.00000	H	–1.65971	0.32289	0.24231
N	4.68041	1.37540	0.00000	N	–0.65561	–0.32182	–4.75095
N	4.86141	–0.84518	0.00000	N	–2.75260	–0.47014	–4.01319
C	5.50563	0.36628	0.00000	C	–1.89824	–0.53063	–5.08507
H	6.58322	0.43786	0.00000	H	–2.25301	–0.73164	–6.08510
H	0.87123	2.84653	0.00000	H	2.17095	0.47991	–1.91445

O	–1.52931	1.63140	0.00000	O	2.04497	0.74834	0.71752
H	5.27201	–1.76339	0.00000	H	–3.75074	–0.59437	–4.01082
H	–4.95869	–2.72969	0.00000	H	–0.33709	–0.44134	5.58445
H	0.15616	0.72238	0.00000	H	0.51216	0.51073	–0.41178
H	–2.51643	–3.49639	0.00000	H	–2.10191	–0.18001	3.74949
Sum of electronic and ZPE corrections:							
	–1009.576579				–1009.576020		
Sum of electronic and thermal free energy:							
	–1009.625849				–1009.626665		
N_{Im} in C_s optimized structure = 1 (282*i* cm^{-1})							

Syn-G•A

	C_s			C_1			
	X	Y	Z		X	Y	Z
C	–2.76630	1.65675	0.00000	C	2.96397	–0.23680	1.13051
C	–2.83672	0.24046	0.00000	C	2.77282	0.05761	–0.23987
N	–1.88567	–0.77286	0.00000	N	1.64832	0.26693	–1.02059
C	–2.58630	–1.87521	0.00000	C	2.11328	0.54976	–2.20820
N	–3.93243	–1.65948	0.00000	N	3.47694	0.52915	–2.26147
C	–4.11705	–0.29898	0.00000	C	3.92327	0.20849	–1.00116
N	–5.27707	0.35564	0.00000	N	5.18351	0.06551	–0.59380
C	–5.07988	1.66978	0.00000	C	5.23357	–0.25289	0.69576
N	–3.92735	2.33667	0.00000	N	4.22669	–0.40406	1.55723
O	1.09327	1.66645	0.00000	O	–0.78022	0.46819	1.82405
C	1.77043	0.65090	0.00000	C	–1.59530	0.24925	0.94129
N	1.14084	–0.60854	0.00000	N	–1.14974	–0.03813	–0.36069
C	3.19436	0.51343	0.00000	C	–3.02676	0.23310	1.00294
C	1.78668	–1.81152	0.00000	C	–1.94529	–0.34392	–1.42194
C	3.73004	–0.76421	0.00000	C	–3.72828	–0.06804	–0.15386
N	3.08668	–1.95233	0.00000	N	–3.24940	–0.38029	–1.38068
N	0.99980	–2.91667	0.00000	N	–1.29220	–0.59131	–2.60531
N	4.19095	1.46595	0.00000	N	–3.88736	0.47101	2.05229
N	5.08067	–0.58102	0.00000	N	–5.04236	–0.00989	0.20437
C	5.29451	0.78232	0.00000	C	–5.07245	0.31959	1.54298
H	6.29129	1.19778	0.00000	H	–6.00459	0.43138	2.07667
N	–1.63008	2.35321	0.00000	N	1.96426	–0.36550	2.01008
H	5.77237	–1.31180	0.00000	H	–5.82515	–0.18039	–0.40450
H	–4.66424	–2.35044	0.00000	H	4.05981	0.71776	–3.06007
H	1.44566	–3.81560	0.00000	H	–1.88529	–0.99939	–3.31074
H	0.00118	–2.84422	0.00000	H	–0.37584	–1.00622	–2.52937
H	0.11230	–0.59471	0.00000	H	–0.13467	0.06484	–0.52369
H	–1.71218	3.35621	0.00000	H	2.22914	–0.50600	2.97121
H	–0.69619	1.94196	0.00000	H	1.01000	–0.05708	1.81844
H	–5.97451	2.28568	0.00000	H	6.22611	–0.40348	1.11006
H	–2.18793	–2.87981	0.00000	H	1.50549	0.78466	–3.07025
Sum of electronic and ZPE corrections:							
	–1009.609454				–1009.611457		
Sum of electronic and thermal free energy:							
	–1009.654233				–1009.657848		
N_{Im} in C_s optimized structure = 2 (391*i* cm^{-1}, 33*i* cm^{-1})							

G•A

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–4.20153	0.81005	0.00000	N	–3.71768	1.14198	–1.59189
C	–4.40813	–0.51324	0.00000	C	–4.28344	0.77844	–0.43391
C	–3.43737	–1.49981	0.00000	C	–3.63435	0.30416	0.69509
C	–2.09052	–1.07509	0.00000	C	–2.23035	0.18753	0.62038
N	–1.85941	0.25687	0.00000	N	–1.64469	0.52736	–0.54718
C	–2.91161	1.08974	0.00000	C	–2.40675	0.98546	–1.55284
H	–2.67283	2.15110	0.00000	H	–1.86364	1.27045	–2.45087
N	–1.07752	–1.93824	0.00000	N	–1.48633	–0.24255	1.64024
N	1.00365	1.12704	0.00000	N	1.18025	–0.06238	–0.83496
C	1.96463	0.09883	0.00000	C	1.92578	–0.13942	0.35435
C	3.29067	0.63399	0.00000	C	3.31846	–0.31746	0.07286
C	3.44102	2.01177	0.00000	C	3.71116	–0.40900	–1.25325
N	2.48800	2.96831	0.00000	N	2.94777	–0.37290	–2.36882
C	1.28008	2.46403	0.00000	C	1.68311	–0.19290	–2.09377
N	0.21267	3.29958	0.00000	N	0.77523	–0.08796	–3.11448
O	1.60533	–1.06994	0.00000	O	1.35799	–0.05301	1.43396
N	4.51720	0.00395	0.00000	N	4.40352	–0.42339	0.91606
C	5.38079	0.97297	0.00000	C	5.42013	–0.57206	0.12189
N	4.78841	2.21948	0.00000	N	5.06402	–0.57268	–1.21048
N	–5.59707	–1.19264	0.00000	N	–5.60869	0.80091	–0.08948
N	–4.00124	–2.75836	0.00000	N	–4.52646	0.04197	1.71367
H	–0.09949	–1.63065	0.00000	H	–0.46354	–0.18694	1.60827
H	0.01754	0.82179	0.00000	H	0.17468	0.16304	–0.72384
H	5.24364	3.11679	0.00000	H	5.66842	–0.67372	–2.00860
H	6.45457	0.85792	0.00000	H	6.44831	–0.68563	0.43203
H	–1.29093	–2.92138	0.00000	H	–1.94613	–0.44231	2.51247
C	–5.28327	–2.53105	0.00000	C	–5.68552	0.34904	1.20639
H	–6.51484	–0.77975	0.00000	H	–6.36754	1.10102	–0.67849
H	–6.05086	–3.29098	0.00000	H	–6.63159	0.26972	1.72152
H	0.38602	4.28798	0.00000	H	1.13576	–0.36278	–4.01394
H	–0.72773	2.95268	0.00000	H	–0.17065	–0.37667	–2.92071
Sum of electronic and ZPE corrections:							
	–1009.612758				–1009.613083		
Sum of electronic and thermal free energy:							
	–1009.657379				–1009.659347		
N_{Im} in C_s optimized structure = 2 (332*i* cm^{-1}, 26*i* cm^{-1})							

G•4-thioU

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	2.46831	–0.09963	0.00000	C	2.46734	–0.03921	0.06887
O	1.58790	–0.95321	0.00000	O	1.59531	–0.03246	0.93062
N	–1.16611	–0.37308	0.00000	N	–1.16448	0.05459	0.38925
C	–1.45706	1.00131	0.00000	C	–1.47022	0.02491	–0.98184
C	–2.86987	1.22146	0.00000	C	–2.88596	0.01917	–1.18611
C	–3.70254	0.11118	0.00000	C	–3.70590	0.03223	–0.06700

N	–3.37569	–1.20017	0.00000	N	–3.36319	0.04909	1.24063
C	–2.08001	–1.38520	0.00000	C	–2.06685	0.06472	1.41064
N	–1.57637	–2.64387	0.00000	N	–1.54754	0.13006	2.66869
O	–0.53906	1.81033	0.00000	O	–0.56214	0.00757	–1.80127
N	–3.60421	2.38810	0.00000	N	–3.63315	–0.00271	–2.34401
C	–4.84097	1.99490	0.00000	C	–4.86561	–0.00198	–1.93675
N	–4.96696	0.62050	0.00000	N	–4.97606	0.01819	–0.56150
H	–0.16578	–0.59893	0.00000	H	–0.16154	0.05809	0.60442
H	–5.81601	0.08059	0.00000	H	–5.81904	0.02507	–0.01215
H	–5.70597	2.64144	0.00000	H	–5.73773	–0.01528	–2.57351
N	2.22980	1.24485	0.00000	N	2.21588	–0.02800	–1.27335
C	3.19028	2.24925	0.00000	C	3.16610	–0.03444	–2.28725
C	4.55835	1.77437	0.00000	C	4.53860	–0.05429	–1.82592
N	3.79438	–0.46039	0.00000	N	3.79684	–0.05921	0.41641
C	4.81712	0.45859	0.00000	C	4.81023	–0.06565	–0.51275
H	1.23094	1.52519	0.00000	H	1.21462	–0.01390	–1.54298
S	2.77501	3.83999	0.00000	S	2.73465	–0.02079	–3.87358
H	5.35361	2.50348	0.00000	H	5.32665	–0.05963	–2.56279
H	3.97596	–1.45075	0.00000	H	3.98815	–0.06378	1.40496
H	5.81876	0.04931	0.00000	H	5.81580	–0.08036	–0.11349
H	–2.22255	–3.41156	0.00000	H	–2.19242	–0.05112	3.41863
H	–0.58685	–2.81517	0.00000	H	–0.58203	–0.11350	2.81502
Sum of electronic and ZPE corrections:							
	–1280.112362				–1280.111712		
Sum of electronic and thermal free energy:							
	–1280.158969				–1280.158432		
N_{Im} in C_s optimized structure = 1 (225*i* cm^{-1})							

G•2-thioU

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	2.78186	–0.21863	0.00000	C	2.71274	0.17419	0.55031
S	1.86412	–1.62684	0.00000	S	1.65366	0.41181	1.83405
N	–1.31511	–0.58339	0.00000	N	–1.34930	0.12031	0.42007
C	–1.45312	0.81485	0.00000	C	–1.34299	0.33529	–0.96852
C	–2.83211	1.19019	0.00000	C	–2.66969	0.27180	–1.49810
C	–3.78250	0.17917	0.00000	C	–3.70979	0.00511	–0.61967
N	–3.60215	–1.15969	0.00000	N	–3.66332	–0.21721	0.71292
C	–2.33595	–1.48962	0.00000	C	–2.44763	–0.13932	1.18632
N	–1.98258	–2.79769	0.00000	N	–2.22967	–0.28533	2.52367
O	–0.45268	1.51844	0.00000	O	–0.28213	0.53920	–1.54154
N	–3.43240	2.43112	0.00000	N	–3.13876	0.42716	–2.78452
C	–4.70503	2.17719	0.00000	C	–4.42217	0.26048	–2.68550
N	–4.98258	0.82511	0.00000	N	–4.83137	–0.00053	–1.39387
H	–0.34494	–0.91276	0.00000	H	–0.43175	0.21070	0.86827
H	–5.88627	0.38261	0.00000	H	–5.76890	–0.16335	–1.06664
H	–5.49309	2.91556	0.00000	H	–5.12720	0.31270	–3.50184
N	2.29692	1.03799	0.00000	N	2.37446	0.15846	–0.75379
C	3.06344	2.23082	0.00000	C	3.25714	–0.03804	–1.84555
C	4.50620	2.01174	0.00000	C	4.65192	–0.22161	–1.45773

N	4.14361	–0.32185	0.00000	N	4.03985	–0.00994	0.81356
C	4.98707	0.76236	0.00000	C	4.98819	–0.19962	–0.16201
H	1.26696	1.17207	0.00000	H	1.38009	0.31554	–1.00895
O	2.52236	3.30625	0.00000	O	2.84163	–0.04247	–2.97555
H	5.15227	2.87652	0.00000	H	5.38215	–0.37016	–2.23872
H	4.50862	–1.26108	0.00000	H	4.29555	0.00207	1.78821
H	6.04395	0.52892	0.00000	H	6.00220	–0.32774	0.19416
H	–2.71585	–3.48291	0.00000	H	–3.00772	–0.64341	3.05124
H	–1.02261	–3.09063	0.00000	H	–1.30764	–0.52720	2.84715
Sum of electronic and ZPE corrections:							
	–1280.107407				–1280.106901		
Sum of electronic and thermal free energy:							
	–1280.152001				–1280.154311		
N_{Im} in C_s optimized structure = 2 (253*i* cm^{-1}, 8*i* cm^{-1})							

G•G 3

	C_s			C_1			
	X	Y	Z		X	Y	Z
N	–2.21946	–3.65198	0.00000	N	–3.14432	0.31581	2.87429
C	–1.29261	–2.58290	0.00000	C	–1.95562	0.21750	2.11428
C	–1.98437	–1.33748	0.00000	C	–2.26015	0.28922	0.72303
C	–3.36525	–1.32396	0.00000	C	–3.57198	0.43068	0.31752
N	–4.21075	–2.37902	0.00000	N	–4.68043	0.50533	1.09053
C	–3.58724	–3.52636	0.00000	C	–4.41174	0.45050	2.36489
N	–4.30738	–4.67472	0.00000	N	–5.42277	0.57614	3.27529
O	–0.09584	–2.80803	0.00000	O	–0.87824	0.09648	2.66781
N	–1.48692	–0.05902	0.00000	N	–1.42080	0.23944	–0.36008
C	–2.52966	0.71942	0.00000	C	–2.19284	0.34452	–1.40295
N	–3.70248	–0.00024	0.00000	N	–3.51587	0.46453	–1.04681
H	–1.79383	–4.56821	0.00000	H	–3.00016	0.33662	3.87422
H	–3.88596	–5.58445	0.00000	H	–5.32146	0.14449	4.17892
H	–5.30860	–4.59514	0.00000	H	–6.34640	0.53110	2.87556
H	–4.63872	0.36996	0.00000	H	–4.30271	0.55877	–1.66788
H	–2.47915	1.79992	0.00000	H	–1.83593	0.33408	–2.42402
N	1.03214	1.25227	0.00000	N	1.34948	–0.07643	–0.90208
C	0.81964	2.64560	0.00000	C	1.53180	–0.13794	–2.29838
C	2.07564	3.34014	0.00000	C	2.91626	–0.35260	–2.60992
C	3.23956	2.58500	0.00000	C	3.81274	–0.46525	–1.55705
N	3.39169	1.24349	0.00000	N	3.58649	–0.40235	–0.22740
C	2.23675	0.61517	0.00000	C	2.31739	–0.20072	0.04896
N	2.20958	–0.73693	0.00000	N	1.92124	–0.08814	1.33845
O	–0.31967	3.08150	0.00000	O	0.56968	–0.01278	–3.03780
N	2.36385	4.68960	0.00000	N	3.56226	–0.47801	–3.82266
C	3.66098	4.74781	0.00000	C	4.80978	–0.66032	–3.51224
N	4.25201	3.50135	0.00000	N	5.02693	–0.66301	–2.14996
H	0.16707	0.69456	0.00000	H	0.37199	0.06091	–0.61125
H	1.35738	–1.28448	0.00000	H	0.94940	–0.04068	1.62081
H	3.09425	–1.21079	0.00000	H	2.61841	–0.25934	2.04032
H	5.23442	3.28561	0.00000	H	5.90035	–0.78306	–1.66578
H	4.25014	5.65301	0.00000	H	5.61899	–0.79851	–4.21407

Sum of electronic and ZPE corrections:							
	–1084.853435				–1084.852896		
Sum of electronic and thermal free energy:							
	–1084.899752				–1084.901676		
N_{Im} in C_s optimized structure = 2 (305*i* cm^{-1}, 16*i* cm^{-1})							

G•6-thioG 3

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–2.43396	–3.78962	0.00000	N	–4.41617	–0.14871	0.86782
C	–1.40936	–2.84222	0.00000	C	–3.02404	–0.12268	0.95388
C	–1.93582	–1.53269	0.00000	C	–2.44245	–0.11685	–0.33361
C	–3.31495	–1.36031	0.00000	C	–3.27111	–0.12925	–1.44843
N	–4.27003	–2.30935	0.00000	N	–4.61794	–0.16917	–1.48016
C	–3.77701	–3.52064	0.00000	C	–5.14967	–0.17406	–0.28772
N	–4.61696	–4.58268	0.00000	N	–6.50655	–0.15847	–0.15128
S	0.17601	–3.34102	0.00000	S	–2.28622	–0.09515	2.44192
N	–1.30549	–0.30898	0.00000	N	–1.12357	–0.08747	–0.72436
C	–2.26250	0.57425	0.00000	C	–1.14768	–0.08133	–2.02698
N	–3.50670	–0.01190	0.00000	N	–2.43069	–0.10682	–2.51985
H	–2.11233	–4.74829	0.00000	H	–4.89119	–0.10287	1.75951
H	–4.29671	–5.53301	0.00000	H	–6.92323	–0.53452	0.68395
H	–5.60369	–4.39509	0.00000	H	–7.01519	–0.31908	–1.00556
H	–4.39636	0.45950	0.00000	H	–2.70564	–0.10660	–3.48848
H	–2.09156	1.64463	0.00000	H	–0.25636	–0.05555	–2.64336
N	1.15927	1.21995	0.00000	N	1.68557	0.00572	–0.00548
C	0.83807	2.59236	0.00000	C	2.44914	0.07509	–1.18824
C	2.03095	3.38695	0.00000	C	3.84573	0.16597	–0.87917
C	3.25390	2.73277	0.00000	C	4.22200	0.17534	0.45565
N	3.51449	1.40890	0.00000	N	3.45100	0.10754	1.56100
C	2.41651	0.68754	0.00000	C	2.17333	0.02013	1.26958
N	2.49936	–0.66019	0.00000	N	1.26308	–0.07707	2.26347
O	–0.33135	2.94323	0.00000	O	1.89160	0.05361	–2.27424
N	2.20394	4.75595	0.00000	N	4.94920	0.25363	–1.70306
C	3.49141	4.92279	0.00000	C	5.95994	0.31386	–0.89043
N	4.18570	3.73039	0.00000	N	5.58341	0.27089	0.43620
H	0.35441	0.58092	0.00000	H	0.66865	–0.04904	–0.14241
H	1.68774	–1.26519	0.00000	H	0.26457	–0.06096	2.09706
H	3.41714	–1.06639	0.00000	H	1.60254	0.00366	3.20480
H	5.18291	3.59842	0.00000	H	6.17868	0.30074	1.24654
H	4.00232	5.87432	0.00000	H	6.99722	0.38989	–1.18147
Sum of electronic and ZPE corrections:							
	–1407.816862				–1407.816332		
Sum of electronic and thermal free energy:							
	–1407.863753				–1407.866059		
N_{Im} in C_s optimized structure = 2 (283*i* cm^{-1}, 3*i* cm^{-1})							

6-thioG•G 3

	C_s				C_1		
	X	Y	Z		X	Y	Z

N	–2.09249	–3.76034	0.00000	N	–3.63240	0.37886	2.28185
C	–1.21210	–2.65466	0.00000	C	–2.33321	0.24957	1.74213
C	–1.94715	–1.43498	0.00000	C	–2.38327	0.28323	0.31806
C	–3.32832	–1.48267	0.00000	C	–3.60526	0.43089	–0.30905
N	–4.13086	–2.57031	0.00000	N	–4.82999	0.53822	0.25603
C	–3.46354	–3.69217	0.00000	C	–4.79013	0.51338	1.55822
N	–4.13667	–4.86842	0.00000	N	–5.94197	0.67288	2.27503
O	–0.00691	–2.83631	0.00000	O	–1.37199	0.13726	2.48228
N	–1.50336	–0.13236	0.00000	N	–1.36801	0.19639	–0.60577
C	–2.58511	0.59339	0.00000	C	–1.95668	0.28728	–1.76481
N	–3.72332	–0.17677	0.00000	N	–3.31717	0.43160	–1.64251
H	–1.62762	–4.65729	0.00000	H	–3.66118	0.42584	3.29084
H	–3.67908	–5.76052	0.00000	H	–6.00592	0.26437	3.19273
H	–5.14031	–4.82921	0.00000	H	–6.78268	0.62789	1.72178
H	–4.67455	0.15296	0.00000	H	–3.98394	0.52011	–2.39171
H	–2.58628	1.67524	0.00000	H	–1.43438	0.24860	–2.71150
N	1.03331	1.34059	0.00000	N	1.54531	–0.14482	–0.66986
C	0.95011	2.72747	0.00000	C	2.13268	–0.25146	–1.92437
C	2.23533	3.32387	0.00000	C	3.53437	–0.43281	–1.82648
C	3.35008	2.49080	0.00000	C	4.10783	–0.47744	–0.55926
N	3.39209	1.14922	0.00000	N	3.50592	–0.36978	0.63573
C	2.18997	0.61012	0.00000	C	2.20416	–0.20004	0.52773
N	2.07255	–0.73167	0.00000	N	1.46490	–0.05943	1.64556
S	–0.52618	3.50562	0.00000	S	1.21867	–0.16372	–3.31803
N	2.62052	4.65001	0.00000	N	4.50021	–0.58291	–2.80187
C	3.91633	4.61614	0.00000	C	5.61136	–0.71292	–2.14716
N	4.42363	3.33083	0.00000	N	5.44129	–0.65779	–0.77694
H	0.14135	0.82770	0.00000	H	0.52490	–0.01593	–0.65104
H	1.19607	–1.24150	0.00000	H	0.45300	0.00080	1.66886
H	2.92828	–1.25677	0.00000	H	1.95391	–0.14657	2.51825
H	5.38928	3.04890	0.00000	H	6.14743	–0.73204	–0.06431
H	4.56691	5.47839	0.00000	H	6.58750	–0.85151	–2.58836
Sum of electronic and ZPE corrections:							
	–1407.817632				–1407.817155		
Sum of electronic and thermal free energy:							
	–1407.864526				–1407.866928		
N_{Im} in C_s optimized structure = 2 (296*i* cm^{-1}, 9*i* cm^{-1})							

G•A 2

	C_s			C_1		
	X	Y	Z	X	Y	Z
N	–3.24620	1.71991	0.00000	3.43747	–0.04637	1.18376
C	–4.44997	0.95392	0.00000	4.47156	0.15671	0.21972
C	–4.13001	–0.44604	0.00000	3.89252	0.55932	–1.03279
C	–2.79792	–0.82136	0.00000	2.51723	0.67694	–1.11742
N	–1.68714	–0.04261	0.00000	1.57702	0.43830	–0.16998
C	–1.96276	1.24266	0.00000	2.09057	0.09088	0.98757
N	–0.96647	2.14714	0.00000	1.27755	–0.11722	2.04511
O	–5.51410	1.52590	0.00000	5.62290	–0.00896	0.54480
N	–4.95467	–1.54945	0.00000	4.48848	0.88672	–2.23108

C	–4.14574	–2.56360	0.00000	C	3.50120	1.19282	–3.01622
N	–2.81782	–2.18572	0.00000	N	2.27236	1.08004	–2.39705
H	–3.40857	2.71669	0.00000	H	3.78588	–0.27090	2.10487
H	–1.16622	3.13021	0.00000	H	1.60668	–0.64860	2.83161
H	0.01076	1.83935	0.00000	H	0.26607	–0.05596	1.89040
H	–2.01676	–2.79324	0.00000	H	1.36964	1.30124	–2.78339
H	–4.43688	–3.60340	0.00000	H	3.58848	1.50430	–4.04641
C	4.47305	–1.60576	0.00000	C	–4.43931	–1.09671	–0.96648
N	3.19720	–1.99948	0.00000	N	–3.20164	–1.14395	–1.46691
C	2.22695	–1.07338	0.00000	C	–2.17261	–0.76076	–0.69775
C	2.61015	0.28452	0.00000	C	–2.45160	–0.34731	0.62227
N	4.95797	–0.36964	0.00000	N	–4.83100	–0.70212	0.23937
C	3.97661	0.53164	0.00000	C	–3.79027	–0.34110	0.98953
N	4.08841	1.90041	0.00000	N	–3.79781	0.10183	2.28968
N	1.90105	1.47313	0.00000	N	–1.65537	0.06864	1.67534
C	2.81745	2.40209	0.00000	C	–2.49551	0.32617	2.63985
H	4.95048	2.41996	0.00000	H	–4.61479	0.22589	2.86432
N	0.95136	–1.48645	0.00000	N	–0.93291	–0.79636	–1.21015
H	2.62598	3.46501	0.00000	H	–2.22275	0.67977	3.62324
H	5.20676	–2.40624	0.00000	H	–5.22609	–1.42050	–1.64122
H	0.14793	–0.85747	0.00000	H	–0.13251	–0.37533	–0.73849
H	0.81026	–2.48221	0.00000	H	–0.84199	–1.11522	–2.15998
Sum of electronic and ZPE corrections:							
		–1009.604372				–1009.604891	
Sum of electronic and thermal free energy:							
		–1009.648796				–1009.652378	
N_{Im} in C_s optimized structure = 2 (132*i* cm^{-1}, 26*i* cm^{-1})							

G•A 4

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	1.30907	–1.95676	0.00000	N	–1.90244	0.18802	–1.34613
C	2.55290	–1.25741	0.00000	C	–2.80024	0.25861	–0.23912
C	2.31069	0.15824	0.00000	C	–2.05240	0.29861	0.98712
C	1.00124	0.60573	0.00000	C	–0.67113	0.26106	0.92130
N	–0.14958	–0.11081	0.00000	N	0.13263	0.16980	–0.16700
C	0.05298	–1.41140	0.00000	C	–0.53490	0.14956	–1.30000
N	–0.99256	–2.25672	0.00000	N	0.12707	0.11652	–2.47414
O	3.58434	–1.88653	0.00000	O	–3.99056	0.28300	–0.44354
N	3.19393	1.21564	0.00000	N	–2.48160	0.38866	2.29314
C	2.44112	2.27219	0.00000	C	–1.39134	0.40541	2.99660
N	1.09447	1.96693	0.00000	N	–0.25367	0.32696	2.21831
H	1.41641	–2.96101	0.00000	H	–2.36881	0.20702	–2.24187
H	–0.84987	–3.24984	0.00000	H	–0.36422	–0.13311	–3.31417
H	–1.95274	–1.88830	0.00000	H	1.14873	–0.00087	–2.46259
H	0.32564	2.61525	0.00000	H	0.70147	0.35457	2.53283
H	2.78856	3.29456	0.00000	H	–1.33616	0.47104	4.07298
C	–4.78225	–2.06875	0.00000	C	3.74467	–0.23716	–3.60631
N	–3.73926	–1.22462	0.00000	N	3.03835	–0.30753	–2.46768
C	–3.97182	0.10003	0.00000	C	3.64081	–0.75702	–1.35256

C	–5.31430	0.52748	0.00000	C	4.99249	–1.14151	–1.44951
N	–6.07357	–1.78628	0.00000	N	5.00827	–0.56489	–3.81557
C	–6.28197	–0.46506	0.00000	C	5.58559	–1.01507	–2.69628
N	–7.47306	0.21182	0.00000	N	6.87313	–1.44589	–2.51305
N	–5.88321	1.78448	0.00000	N	5.88202	–1.63475	–0.51722
C	–7.16446	1.55091	0.00000	C	6.98428	–1.80164	–1.19032
H	–8.38952	–0.20419	0.00000	H	7.58901	–1.48683	–3.21931
N	–2.94460	0.95688	0.00000	N	2.95176	–0.82825	–0.20762
H	–7.93524	2.30765	0.00000	H	7.91103	–2.17892	–0.78342
H	–4.52374	–3.12396	0.00000	H	3.19895	0.13988	–4.46667
H	–3.14831	1.94141	0.00000	H	3.42106	–1.17610	0.61064
H	–1.97868	0.61937	0.00000	H	1.98991	–0.48497	–0.15552
Sum of electronic and ZPE corrections:							
	–1009.606570				–1009.606146		
Sum of electronic and thermal free energy:							
	–1009.650784				–1009.654054		
N_{Im} in C_s optimized structure = 2 (83*i* cm^{-1}, 9*i* cm^{-1})							

8-oxoG•G

	C_s			C_1			
	X	Y	Z		X	Y	Z
N	–2.65435	0.77097	0.00000	N	–2.17019	0.22456	–1.70470
C	–2.55469	–0.62797	0.00000	C	–2.59128	0.22179	–0.36665
C	–3.85293	–1.22890	0.00000	C	–4.01872	0.26688	–0.28391
C	–4.95954	–0.39084	0.00000	C	–4.74048	0.28999	–1.46912
N	–5.00809	0.95909	0.00000	N	–4.28933	0.27905	–2.74256
C	–3.81131	1.49246	0.00000	C	–2.98159	0.24986	–2.79970
N	–3.66462	2.83882	0.00000	N	–2.34981	0.27435	–4.00294
O	–1.45009	–1.15761	0.00000	O	–1.75991	0.18150	0.53201
N	–4.23767	–2.55309	0.00000	N	–4.86194	0.28391	0.80676
C	–5.53493	–2.51606	0.00000	C	–6.05482	0.31769	0.29641
N	–6.03480	–1.22964	0.00000	N	–6.04804	0.32247	–1.08345
H	–1.76577	1.29153	0.00000	H	–1.15346	0.17618	–1.86179
H	–2.75294	3.26364	0.00000	H	–1.36851	0.05318	–4.05376
H	–4.49184	3.40639	0.00000	H	–2.92118	0.11723	–4.81432
H	–6.99955	–0.94427	0.00000	H	–6.84059	0.34843	–1.70269
H	–6.18823	–3.37600	0.00000	H	–6.97765	0.34050	0.85691
C	3.02594	–1.13579	0.00000	C	2.38975	–0.11814	2.17892
C	2.29127	0.08213	0.00000	C	2.15785	–0.12578	0.77418
N	0.92435	0.34667	0.00000	N	0.99140	–0.02705	0.02280
C	0.72660	1.69088	0.00000	C	1.30288	–0.06896	–1.29984
N	1.99099	2.26306	0.00000	N	2.68361	–0.19421	–1.36268
C	2.95277	1.28348	0.00000	C	3.21203	–0.22755	–0.09618
N	4.28372	1.50239	0.00000	N	4.52440	–0.34997	0.19710
C	4.98551	0.39850	0.00000	C	4.76614	–0.34323	1.48011
N	4.42361	–0.84423	0.00000	N	3.78995	–0.23799	2.42550
N	6.33988	0.47441	0.00000	N	6.05929	–0.39804	1.92318
O	–0.33645	2.31395	0.00000	O	0.54790	–0.01103	–2.27123
H	0.14499	–0.33000	0.00000	H	0.01979	0.05536	0.36154
H	5.00485	–1.67046	0.00000	H	4.03506	–0.17611	3.40380

H	6.93067	–0.33554	0.00000	H	6.24214	–0.80341	2.82633
H	6.75449	1.38896	0.00000	H	6.72895	–0.62656	1.20605
O	2.64921	–2.28659	0.00000	O	1.61615	–0.02516	3.10537
H	2.15122	3.25590	0.00000	H	3.19813	–0.24387	–2.22541
Sum of electronic and ZPE corrections:							
		–1160.103732				–1160.102877	
Sum of electronic and thermal free energy:							
		–1160.152995				–1160.152745	
N_{Im} in C_s optimized structure = 2 (313*i* cm^{-1}, 156*i* cm^{-1})							

1

	C_s			C_1			
	X	Y	Z		X	Y	Z
N	0.18923	–0.48124	0.00000	N	0.29525	0.28268	–0.41752
C	–0.20128	–1.79172	0.00000	C	0.38889	–0.16985	–1.70616
C	–0.63386	0.66059	0.00000	C	–0.78546	0.04748	0.45077
N	0.10905	1.82100	0.00000	N	–0.35943	–0.10129	1.76936
O	0.58255	–2.70988	0.00000	O	1.29218	0.11614	–2.45328
H	–0.35853	2.70727	0.00000	H	–1.10478	–0.24320	2.43368
H	1.11075	1.81963	0.00000	H	0.39919	–0.75703	1.89535
H	–1.29038	–1.93584	0.00000	H	–0.44132	–0.83969	–1.98266
H	1.19083	–0.35377	0.00000	H	1.05904	0.85389	–0.08214
C	–1.97454	0.64017	0.00000	C	–2.05764	0.02987	0.03970
H	–2.52108	1.57305	0.00000	H	–2.84867	–0.27813	0.71067
H	–2.54570	–0.27376	0.00000	H	–2.32735	0.34944	–0.95667
Sum of electronic and ZPE corrections:							
		–302.536089				–302.541627	
Sum of electronic and thermal free energy:							
		–302.565545				–302.571577	
N_{Im} in C_s optimized structure = 2 (490*i* cm^{-1}, 200*i* cm^{-1})							

2

	C_s			C_1			
	X	Y	Z		X	Y	Z
N	1.57780	0.98327	0.00000	N	1.43304	–0.11198	–1.19919
C	1.93137	–0.33839	0.00000	C	1.96285	0.08073	0.04808
C	2.42918	2.09364	0.00000	C	2.10707	0.03290	–2.41817
H	1.87945	3.02837	0.00000	H	1.44682	0.27092	–3.24566
O	1.12917	–1.24020	0.00000	O	1.34838	–0.09603	1.07141
H	0.58280	1.15161	0.00000	H	0.44840	–0.33361	–1.21690
H	3.01846	–0.50815	0.00000	H	3.00556	0.43586	0.02507
C	3.75978	2.10942	0.00000	C	3.41766	–0.08335	–2.61321
H	4.26858	3.06347	0.00000	H	3.82550	0.10410	–3.59717
H	4.37646	1.22009	0.00000	H	4.11074	–0.36162	–1.82889
Sum of electronic and ZPE corrections:							
		–247.193935				–247.194049	
Sum of electronic and thermal free energy:							
		–247.221647				–247.222514	
N_{Im} in C_s optimized structure = 1 (100*i* cm^{-1})							

5

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	2.44238	2.14995	0.00000	C	2.31579	–0.23367	–2.27965
N	1.61902	1.01280	0.00000	N	1.60757	0.03099	–1.10741
C	2.13137	–0.15484	0.00000	C	2.09896	–0.35807	–0.00009
N	1.36179	–1.26910	0.00000	N	1.56582	–0.00705	1.20323
H	1.85938	3.06684	0.00000	H	1.69734	–0.61116	–3.09060
H	1.76685	–2.18593	0.00000	H	1.77451	–0.56569	2.01165
H	0.36039	–1.16848	0.00000	H	0.67730	0.46820	1.18970
H	3.20611	–0.36685	0.00000	H	2.99694	–0.98430	0.06250
C	3.77441	2.24825	0.00000	C	3.61430	0.00080	–2.48161
H	4.23676	3.22721	0.00000	H	4.06984	–0.21496	–3.44007
H	4.44522	1.39551	0.00000	H	4.23774	0.44985	–1.71522
Sum of electronic and ZPE corrections:							
		–227.291863				–227.295853	
Sum of electronic and thermal free energy:							
		–227.319413				–227.324091	
N_{Im} in C_s optimized structure = 2 (226*i* cm^{-1}, 138*i* cm^{-1})							

6

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	1.36079	1.19382	0.00000	C	–1.72221	0.14567	0.15835
N	0.54164	2.27188	0.00000	N	–1.88529	–0.17128	1.46978
N	0.90475	0.00583	0.00000	N	–0.80755	–0.37222	–0.56046
C	1.78394	–1.09770	0.00000	C	–0.81673	–0.08756	–1.93285
N	1.04913	–2.25993	0.00000	N	0.43947	0.30633	–2.38679
C	3.13093	–1.07890	0.00000	C	–1.90516	–0.18393	–2.71576
H	0.90769	3.20491	0.00000	H	–2.42309	0.43595	2.06158
H	–0.45452	2.13073	0.00000	H	–1.17732	–0.74067	1.90485
H	2.42441	1.44903	0.00000	H	–2.45300	0.85814	–0.23839
H	1.49140	–3.15873	0.00000	H	0.61551	0.14206	–3.36534
H	0.04918	–2.19131	0.00000	H	1.19034	–0.00803	–1.79174
H	3.69267	–2.00404	0.00000	H	–1.85292	0.03015	–3.77608
H	3.69932	–0.16055	0.00000	H	–2.84588	–0.52860	–2.31028
Sum of electronic and ZPE corrections:							
		–282.641376				–282.644677	
Sum of electronic and thermal free energy:							
		–282.670384				–282.674736	
N_{Im} in C_s optimized structure = 3 (393*i* cm^{-1}, 160*i* cm^{-1}, 131*i* cm^{-1})							

1•1

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.30964	0.45144	0.00000	C	0.05093	–0.01978	–0.50437
O	–0.47457	1.39422	0.00000	O	1.24825	–0.11340	–0.74495
N	–3.28095	0.83145	0.00000	N	3.04166	–0.08029	1.47749
C	–3.67558	–0.45144	0.00000	C	2.49447	0.08309	2.69660
C	–4.09436	1.98558	0.00000	C	4.39435	0.15633	1.15874

N	–3.31444	3.11580	0.00000	N	4.53663	0.81894	–0.05168
O	–2.89137	–1.39422	0.00000	O	1.30777	–0.10043	2.93799
H	–2.26709	0.99217	0.00000	H	2.39618	–0.24836	0.69641
N	–0.08499	–0.83145	0.00000	N	–0.48243	–0.21746	0.71579
C	0.72842	–1.98558	0.00000	C	–1.84933	–0.08316	1.03346
H	–1.09885	–0.99217	0.00000	H	0.17383	–0.33114	1.49769
N	–0.05149	–3.11580	0.00000	N	–2.04215	0.57363	2.24005
H	–3.74796	4.01890	0.00000	H	5.39643	0.64066	–0.54388
H	–2.31041	3.06228	0.00000	H	3.72519	0.82828	–0.65190
H	0.38202	–4.01890	0.00000	H	–2.88590	0.33295	2.73347
H	–1.05552	–3.06228	0.00000	H	–1.23394	0.64850	2.84003
H	–4.75955	–0.61511	0.00000	H	3.20287	0.40676	3.47140
H	1.39361	0.61511	0.00000	H	–0.67998	0.24427	–1.28087
C	2.06966	–1.98215	0.00000	C	–2.82417	–0.50947	0.22116
H	2.60681	–2.92043	0.00000	H	–3.86066	–0.30332	0.45170
H	2.65047	–1.07359	0.00000	H	–2.59854	–1.07912	–0.66816
C	–5.43559	1.98215	0.00000	C	5.39876	–0.18945	1.97328
H	–5.97275	2.92043	0.00000	H	6.41650	0.09403	1.74131
H	–6.01640	1.07359	0.00000	H	5.21718	–0.76952	2.86594
Sum of electronic and ZPE corrections:							
		–605.103357				–605.105947	
Sum of electronic and thermal free energy:							
		–605.143687				–605.148809	
N_{Im} in C_s optimized structure = 4 (345i cm^{-1}, 339i cm^{-1}, 129i cm^{-1}, 103i cm^{-1})							

2•2

	C_s			C_1			
	X	Y	Z		X	Y	Z
N	–1.62436	–0.94032	0.00000	N	–1.55065	0.03910	1.04981
N	1.61223	0.95170	0.00000	N	1.54104	–0.04076	–1.06061
C	–2.01286	0.35094	0.00000	C	–2.00244	0.30215	–0.19347
C	2.00074	–0.33956	0.00000	C	1.99283	–0.30377	0.18267
C	–2.45988	–2.06454	0.00000	C	–2.34200	–0.00813	2.20558
C	2.44774	2.07592	0.00000	C	2.33238	0.00637	–2.21639
H	–1.88831	–2.98574	0.00000	H	–1.78251	0.21791	3.10686
H	1.87617	2.99712	0.00000	H	1.77287	–0.21968	–3.11766
O	–1.23867	1.29625	0.00000	O	–1.30175	0.30140	–1.19445
O	1.22655	–1.28487	0.00000	O	1.29216	–0.30291	1.18367
H	–0.61142	–1.10546	0.00000	H	–0.53580	–0.08314	1.15163
H	0.59929	1.11683	0.00000	H	0.52619	0.08156	–1.16242
H	–3.09957	0.51077	0.00000	H	–3.07403	0.54408	–0.24565
C	–3.78989	–2.10548	0.00000	C	–3.63956	–0.29422	2.26452
H	–4.28139	–3.06866	0.00000	H	–4.14944	–0.25510	3.21760
H	–4.42466	–1.22847	0.00000	H	–4.22379	–0.57596	1.39672
H	3.08744	–0.49939	0.00000	H	3.06440	–0.54577	0.23485
C	3.77776	2.11688	0.00000	C	3.62996	0.29240	–2.27536
H	4.26925	3.08006	0.00000	H	4.13983	0.25321	–3.22844
H	4.41254	1.23986	0.00000	H	4.21421	0.57416	–1.40758
Sum of electronic and ZPE corrections:							
		–494.410697				–494.410992	

Sum of electronic and thermal free energy:							
	–494.448542				–494.450662		
N_{Im} in C_s optimized structure = 2 (89*i* cm^{-1}, 82*i* cm^{-1})							

5•5

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–2.85142	1.50698	0.00000	C	2.17754	–0.17288	2.38828
N	–1.77025	0.61474	0.00000	N	1.44637	–0.33481	1.21027
C	–1.98151	–0.65731	0.00000	C	2.08978	–0.39135	0.09763
N	–0.99025	–1.55394	0.00000	N	1.49313	–0.41005	–1.10230
H	–2.51853	2.54235	0.00000	H	1.82701	–0.79048	3.21289
H	–1.21200	–2.53260	0.00000	H	2.04715	–0.56458	–1.92429
H	0.00000	–1.25431	0.00000	H	0.46762	–0.37579	–1.18520
C	2.85142	–1.50698	0.00000	C	–2.18033	–0.14118	–2.38582
N	1.77024	–0.61473	0.00000	N	–1.45552	–0.30517	–1.20418
C	1.98150	0.65731	0.00000	C	–2.10017	–0.31183	–0.09083
N	0.99025	1.55394	0.00000	N	–1.50418	–0.32699	1.10947
H	2.51852	–2.54234	0.00000	H	–1.85445	–0.79015	–3.19633
H	1.21200	2.53260	0.00000	H	–2.06345	–0.44153	1.93446
H	0.00000	1.25431	0.00000	H	–0.47809	–0.33087	1.19204
H	2.98646	1.09048	0.00000	H	–3.19605	–0.31576	–0.07357
C	4.16761	–1.27644	0.00000	C	–3.15420	0.74653	–2.60114
H	4.85342	–2.11383	0.00000	H	–3.64932	0.79654	–3.56293
H	4.61083	–0.28667	0.00000	H	–3.45536	1.46008	–1.84106
H	–2.98646	–1.09048	0.00000	H	3.18467	–0.43831	0.08092
C	–4.16761	1.27644	0.00000	C	3.18530	0.68084	2.58419
H	–4.85343	2.11383	0.00000	H	3.68243	0.73294	3.54483
H	–4.61083	0.28667	0.00000	H	3.51366	1.36502	1.80854
Sum of electronic and ZPE corrections:							
	–454.606657				–454.614236		
Sum of electronic and thermal free energy:							
	–454.644965				–454.654359		
N_{Im} in C_s optimized structure = 2 (186*i* cm^{-1}, 181*i* cm^{-1})							

3•1

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	3.68235	–2.88165	0.00000	C	–4.10962	–0.38135	–2.16625
O	3.00743	–3.88501	0.00000	O	–3.63189	–0.24595	–3.26843
N	0.24392	–1.16091	0.00000	N	–0.47113	–0.03131	–1.10527
C	–0.04398	0.14888	0.00000	C	0.02269	0.28939	0.10218
C	–0.67582	–2.23523	0.00000	C	0.24148	0.01439	–2.32135
N	–0.02479	–3.43940	0.00000	N	–0.55445	0.41474	–3.38022
O	0.80694	1.03324	0.00000	O	–0.62242	0.22021	1.14336
H	1.24673	–1.38925	0.00000	H	–1.48469	–0.20965	–1.13789
N	3.14590	–1.61750	0.00000	N	–3.36153	–0.33005	–1.01543
C	3.98746	–0.62402	0.00000	C	–3.99771	–0.45084	0.11329
N	3.58606	0.63343	0.00000	N	–3.37426	–0.38473	1.27566
H	–0.56854	–4.28133	0.00000	H	–0.20833	0.14673	–4.28717

H	0.98373	–3.53052	0.00000	H	–1.55603	0.27036	–3.29216
H	4.25748	1.38086	0.00000	H	–3.88888	–0.47322	2.13404
H	2.57504	0.84720	0.00000	H	–2.35865	–0.19626	1.30051
H	–1.11131	0.39921	0.00000	H	1.06555	0.63431	0.09532
H	4.79207	–2.95001	0.00000	H	–5.20096	–0.55442	–2.04127
C	–2.01228	–2.09155	0.00000	C	1.55177	–0.26168	–2.40015
H	–2.64180	–2.97071	0.00000	H	2.07955	–0.14054	–3.33657
H	–2.49925	–1.12960	0.00000	H	2.10556	–0.61941	–1.54506
H	5.07199	–0.78630	0.00000	H	–5.08172	–0.61183	0.15262
Sum of electronic and ZPE corrections:							
		–565.831745				–565.832518	
Sum of electronic and thermal free energy:							
		–565.869423				–565.871937	
N_{Im} in C_s optimized structure = 2 (180*i* cm^{-1}, 80*i* cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
C	–2.59384	–1.53915	0.00000	C	2.95324	–0.10387	–0.30994
C	1.32910	1.18867	0.00000	C	–1.64572	0.41394	0.48949
O	–1.96452	–2.56611	0.00000	O	2.81056	0.17276	–1.47428
N	0.57127	2.29518	0.00000	N	–1.47277	0.36075	1.81999
N	–2.02179	–0.28893	0.00000	N	1.90916	–0.26468	0.56776
N	0.84832	–0.00282	0.00000	N	–0.74235	0.05833	–0.35235
C	–2.78382	0.84533	0.00000	C	2.09848	–0.52256	1.89549
C	1.74804	–1.10339	0.00000	C	–1.09439	0.02464	–1.71624
H	–0.97180	–0.20722	0.00000	H	0.92421	–0.16187	0.20498
O	–2.33448	1.96849	0.00000	O	1.20010	–0.60683	2.70216
N	1.06411	–2.29064	0.00000	N	–0.12859	0.60050	–2.52775
H	–3.87032	0.65600	0.00000	H	3.15532	–0.64742	2.18635
H	–3.69742	–1.52374	0.00000	H	3.94855	–0.24746	0.14588
C	3.09548	–1.04479	0.00000	C	–2.24793	–0.50171	–2.16585
H	1.01157	3.19642	0.00000	H	–2.17718	0.73003	2.43094
H	–0.44509	2.24813	0.00000	H	–0.61469	–0.00878	2.22163
H	2.40195	1.38631	0.00000	H	–2.61791	0.78384	0.15327
H	1.57376	–3.15377	0.00000	H	–0.16928	0.32096	–3.49502
H	0.05726	–2.33466	0.00000	H	0.81605	0.58264	–2.16272
H	3.67382	–1.95940	0.00000	H	–2.48205	–0.50815	–3.22297
H	3.65175	–0.12020	0.00000	H	–2.94493	–0.97356	–1.48806
Sum of electronic and ZPE corrections:							
		–565.827803				–565.831879	
Sum of electronic and thermal free energy:							
		–565.865411				–565.871293	
N_{Im} in C_s optimized structure = 2 (208*i* cm^{-1}, 114*i* cm^{-1})							