Electronic Supporting Information

Aromaticity Gain Increases the Inherent Association Strengths of Multipoint Hydrogen-Bonded Arrays

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Details of computational methods

All array monomers and complexes were constrained to C_s symmetry and optimized using an ultrafine grid in the gas-phase at ωB97X-D/6-311+G(d,p) and in implicit chloroform solvation at IEF-PCM-ωB97X-D/6-311+G(d,p). Negative values of the computed association free energies ($-\Delta G_{assoc}$) for each hydrogen-bonded complex are tabulated in Tables S1-S8. Vibrational frequency calculations verified the nature of the stationary points. For monomers with a nonplanar C_1 minima, planarization energies were computed in the gas-phase at ωB97X-D/6-31+G(d) (see Table S9). All geometry optimizations were performed employing the Gaussian09 program.

Block-localized wavefunction (BLW)

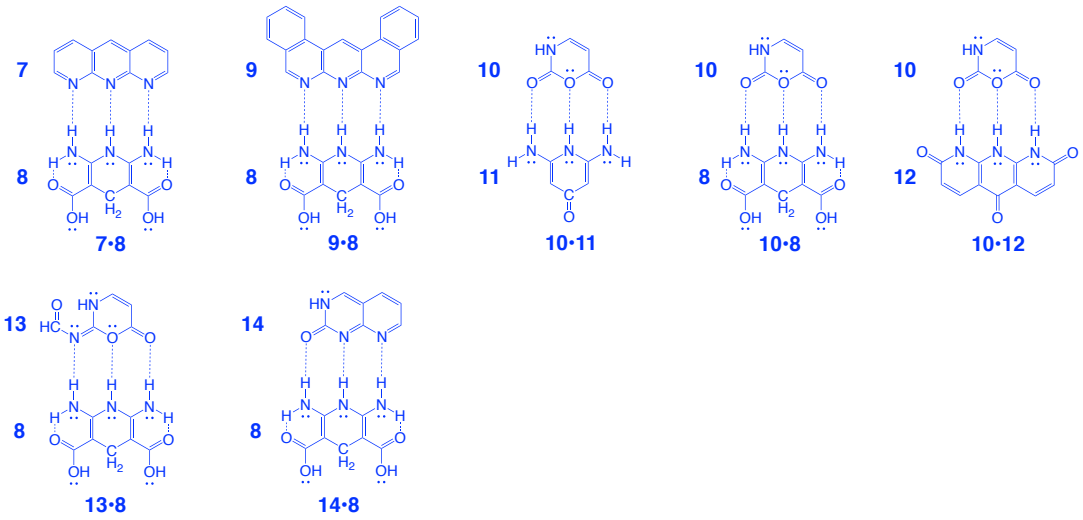
BLW computations quantified the π-electron delocalization energies (DE_π) of all triply and quadruply hydrogen-bonded complexes (A•B) and their individual hydrogen-bonding monomers (A and B). For each monomer or complex considered, DE_π values were calculated by the energy difference between the fully delocalized wavefunction (ψ_{deloc}) and the energy of a π-electron-localized wavefunction (ψ_{loc}); $DE_\pi = E(\psi_{loc}) - E(\psi_{deloc})$. 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.

Based on the computed DE_π values of each complex (A•B) and its individual monomers (A and B), ΔDE_π provides a measure of the π-conjugation gain in the array monomers upon hydrogen bonding to give the complex; $\Delta DE_\pi = DE_{\pi(A\bullet B)} - [DE_{\pi(A)} + DE_{\pi(B)}]$. For a given complex, a large ΔDE_π value indicates significant π-conjugation gain and suggests increased aromatic character in the monomers upon hydrogen bonding. A small ΔDE_π value indicates negligible π-conjugation gain and suggests little to no aromaticity gain in the monomers upon hydrogen bonding. BLW computations were carried out in the gas-phase at B3LYP/6-31G(d//ωB97X-D/6-311+G(d,p) and in implicit chloroform solvation at PCM-B3LYP/6-31G(d)//IEF-PCM-ωB97X-D/6-311+G(d,p) based on the fully planar geometries of all monomers and complexes. All BLW computations were performed employing the GAMESS 2013-R1 program.

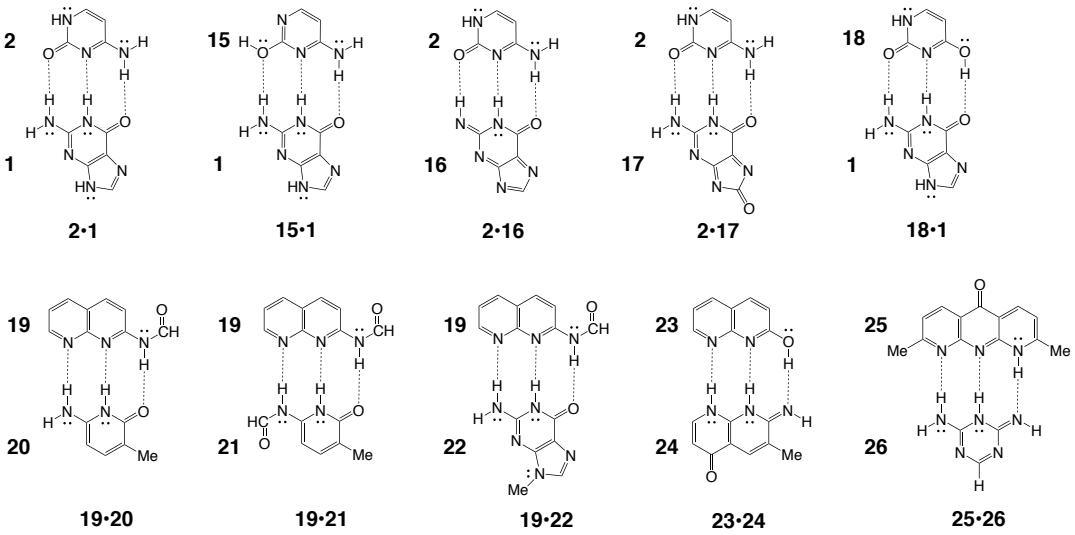
Natural bond orbital deletion (NBO-DEL)

Natural bond orbital (NBO) computations were performed at ωB97X-D/Def2-TZVPP// ωB97X-D/6-311+G(d,p) in the gas-phase and in implicit chloroform solvation, using the fully planar geometries of all monomers and complexes. Using the NBO deletion keyword, all π* orbitals were deleted to quantify the effects of π-electron delocalization (DEL_π) for each of the complexes (A•B) and their individual monomers (A and B). ΔNBO-DEL_π is the computed DEL_π of the complex minus that of its monomers, and provides a measure of the degree of increased π-electron delocalization in the monomers upon hydrogen bonding; $\Delta\text{NBO-}DEL_\pi = DEL_{\pi(A\bullet B)} - [DEL_{\pi(A)} + DEL_{\pi(B)}]$.

AAA–DDD



ADD–DAA



ADA–DAD

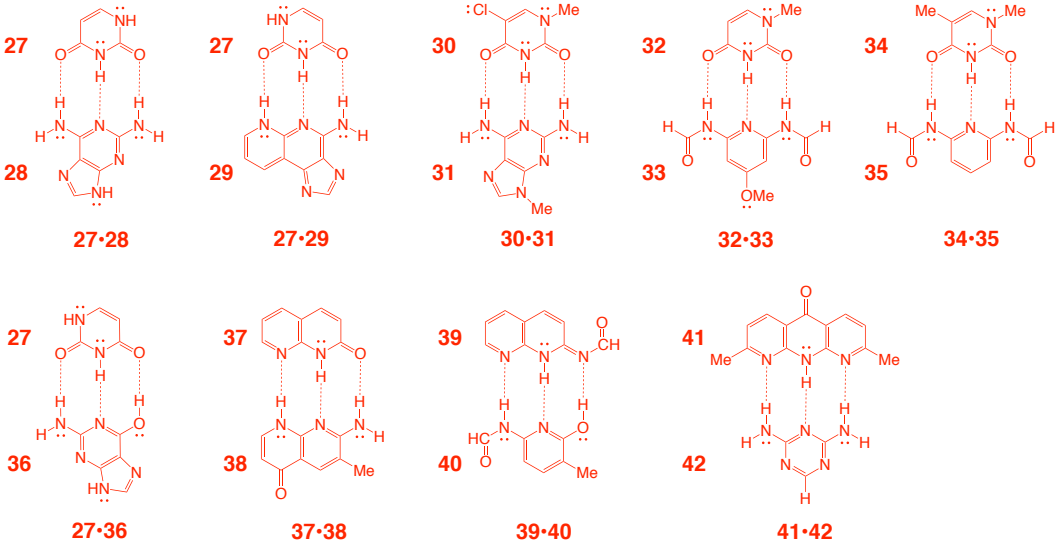
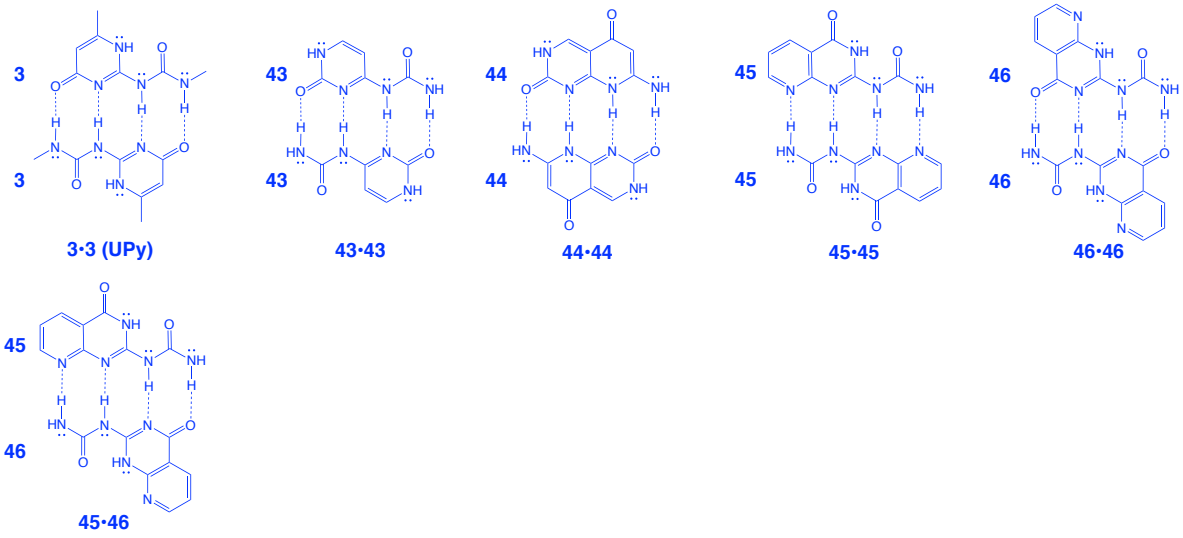
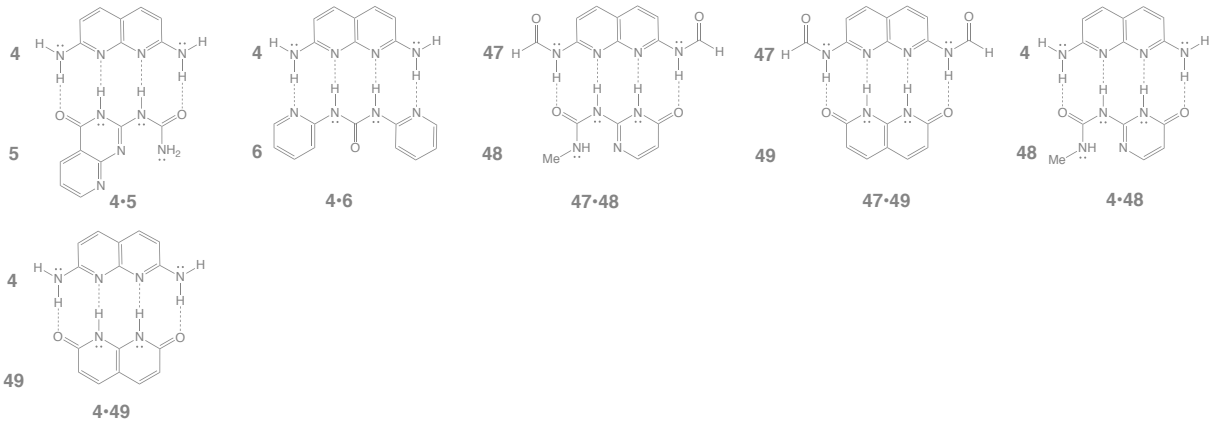


Figure S1. Structures for all triply hydrogen-bonded arrays considered.

AADD–DDAA



ADDA–DAAD



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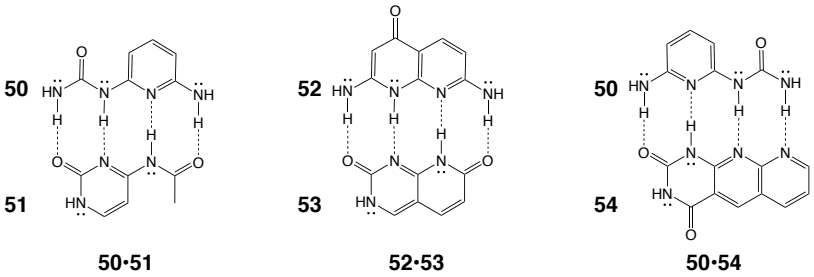

ADAD–DADA

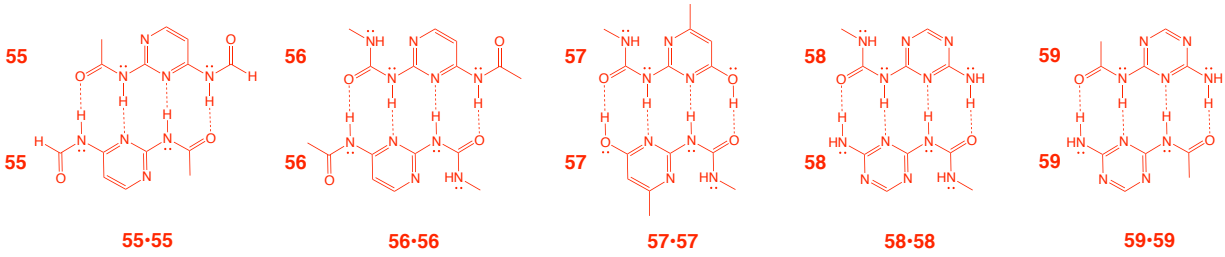

Figure S2. Structures for all quadruply hydrogen-bonded arrays considered.

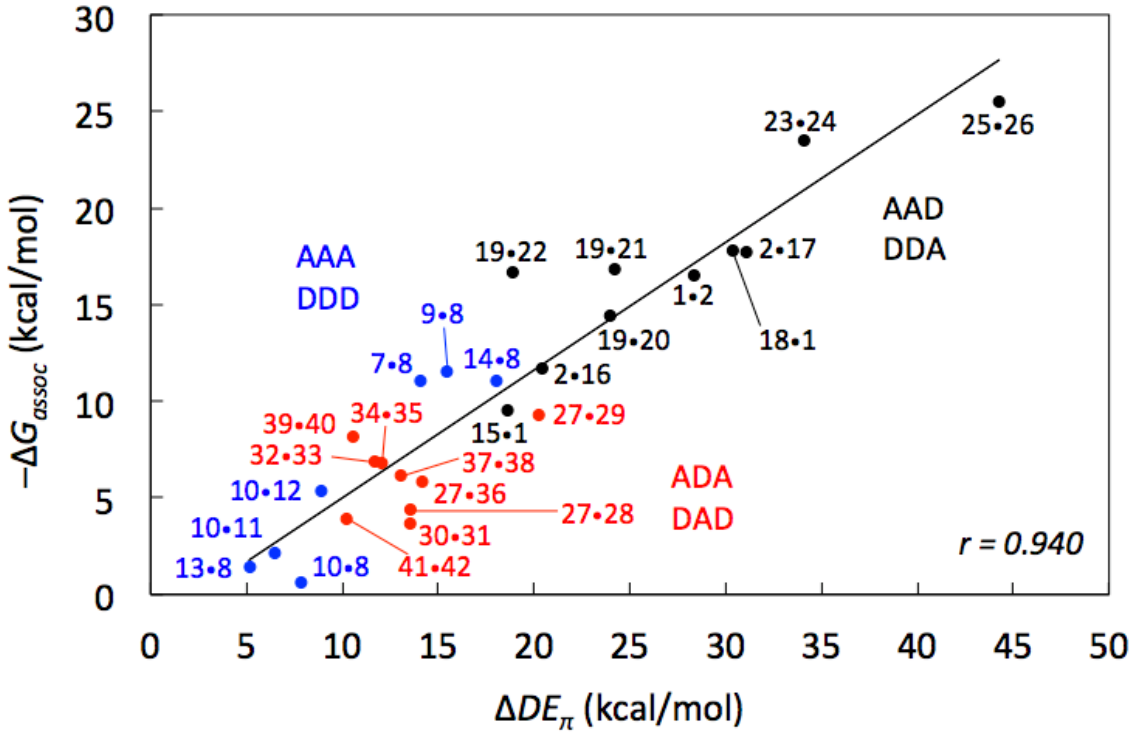

Figure S3. Plot of $-\Delta G_{assoc}$ vs. ΔDE_{π} for triply hydrogen-bonded arrays in the gas-phase. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. BLW computations were performed at B3LYP/6-31G(d).

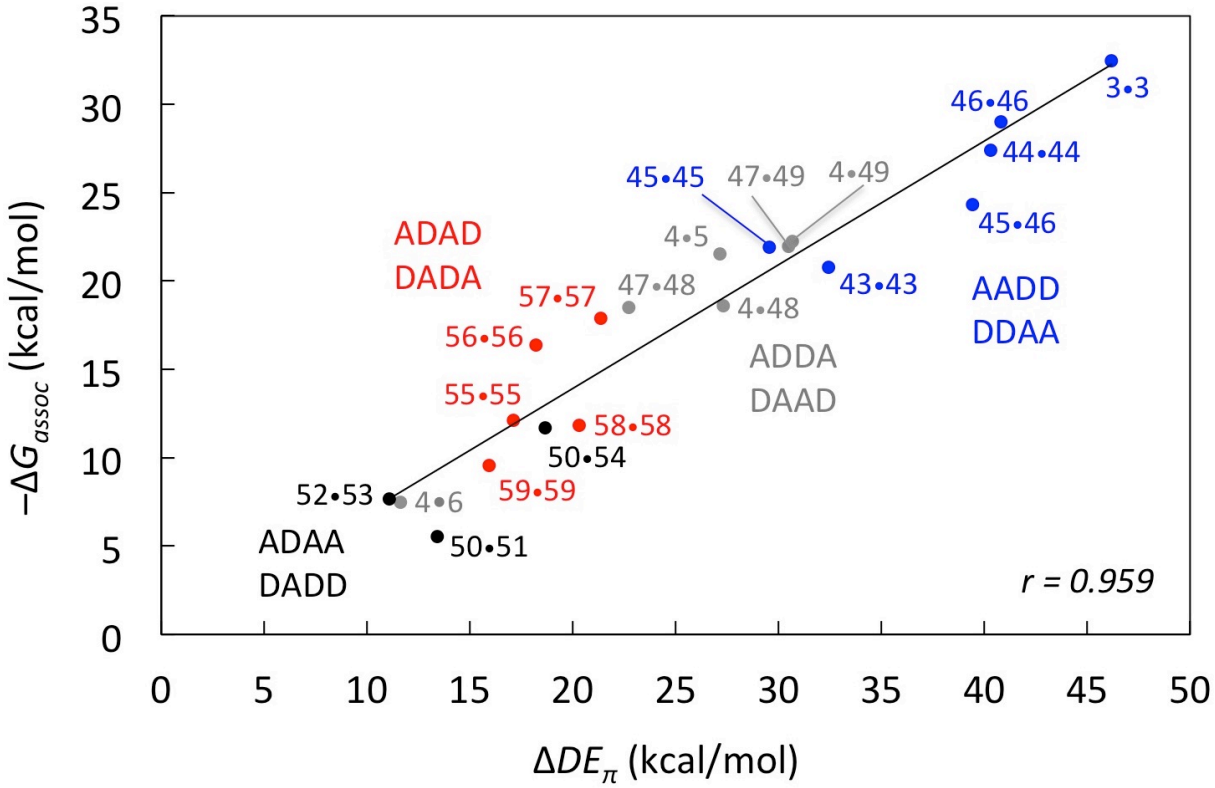

Figure S4. Plot of $-\Delta G_{assoc}$ vs. ΔDE_{π} for quadruply hydrogen-bonded arrays in the gas-phase. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. BLW computations were performed at B3LYP/6-31G(d).

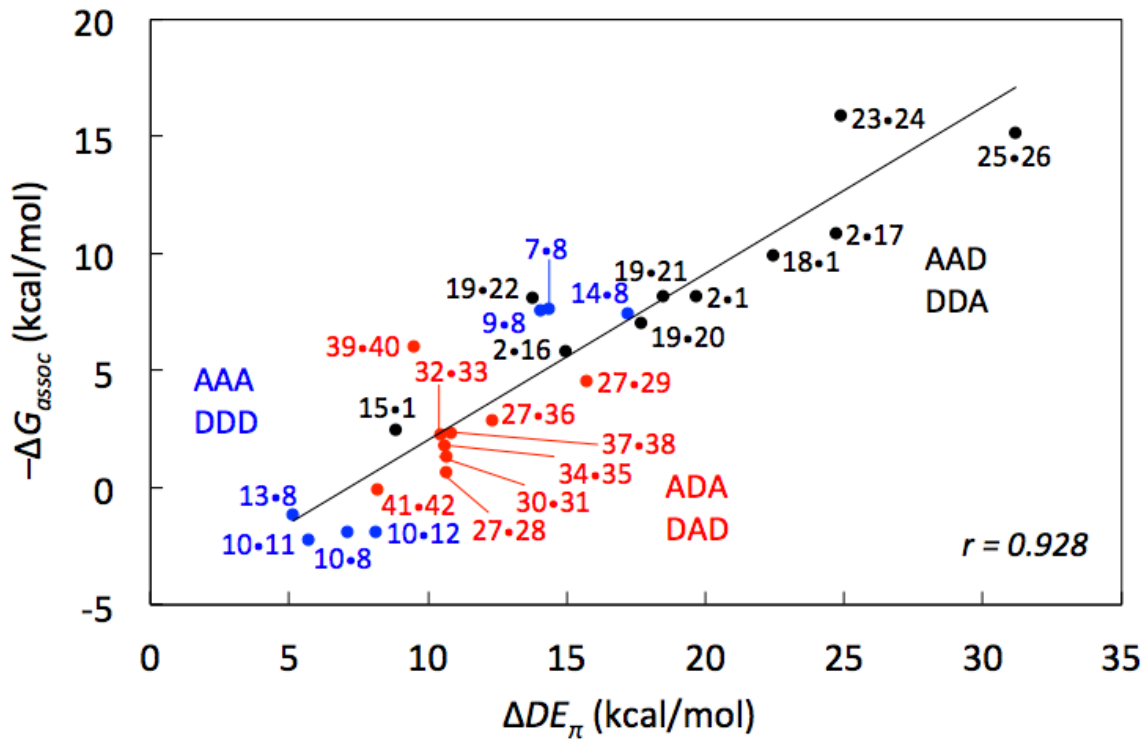

Figure S5. Plot of $-\Delta G_{assoc}$ vs. ΔDE_{π} for triply hydrogen-bonded arrays in implicit chloroform solvation. All geometries were optimized with C_s symmetry at the IEF-PCM-ωB97X-D/6-311+G(d,p) level. BLW computations were performed in implicit chloroform solvation at PCM-B3LYP/6-31G(d).

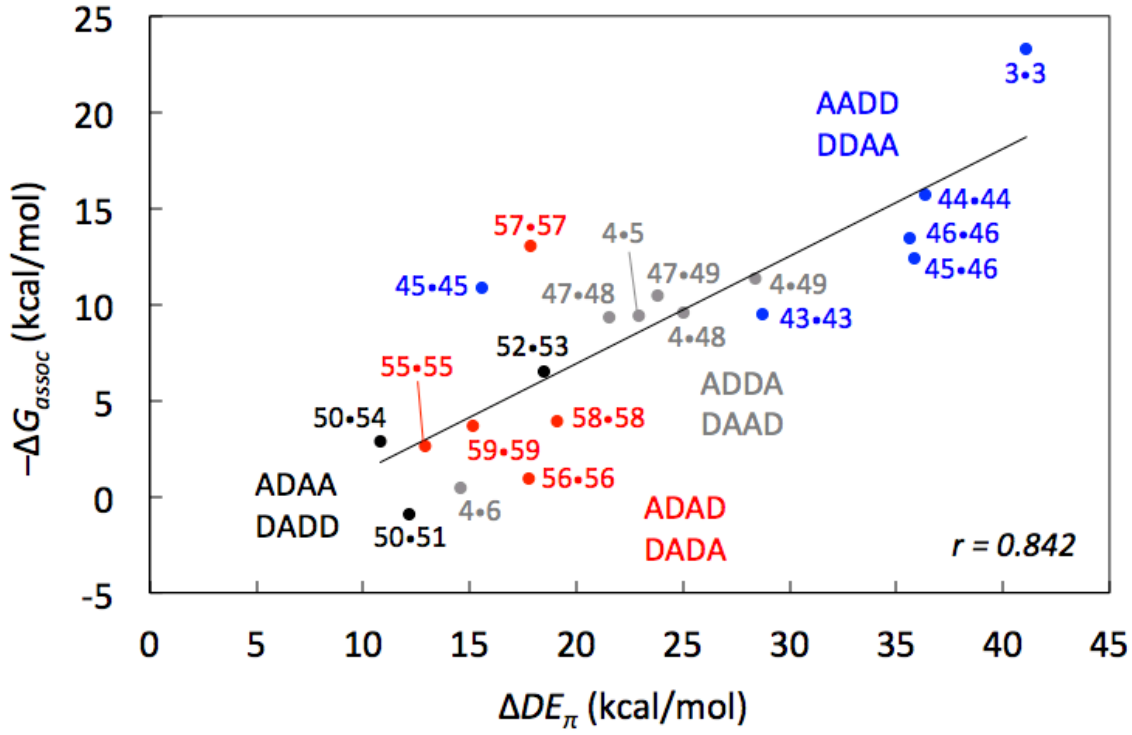

Figure S6. Plot of $-\Delta G_{\text{assoc}}$ vs. ΔDE_{π} for quadruply hydrogen-bonded arrays in implicit chloroform solvation. All geometries were optimized with C_s symmetry at the IEF-PCM-ωB97X-D/6-311+G(d,p) level. BLW computations were performed in implicit chloroform solvation at PCM-B3LYP/6-31G(d).

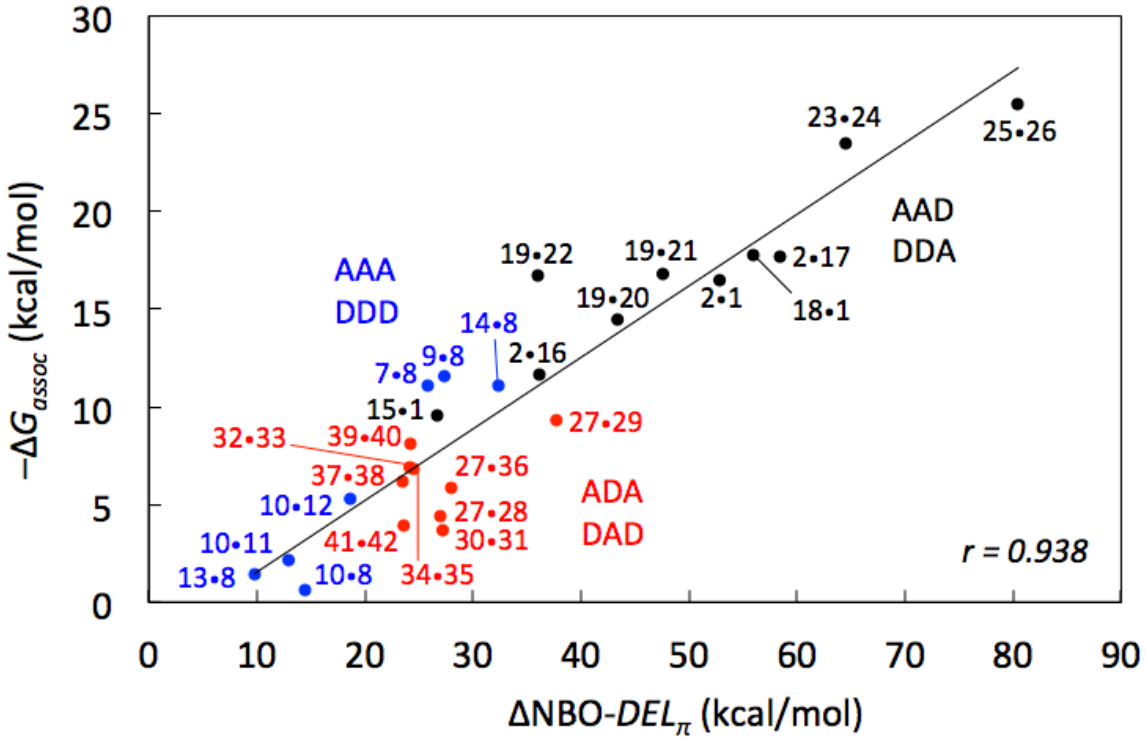

Figure S7. Plot of $-\Delta G_{assoc}$ vs. ΔNBO-DEL_{π} for triply hydrogen-bonded arrays in the gas-phase. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. NBO deletion computations were performed at ωB97X-D/def2-TZVPP.

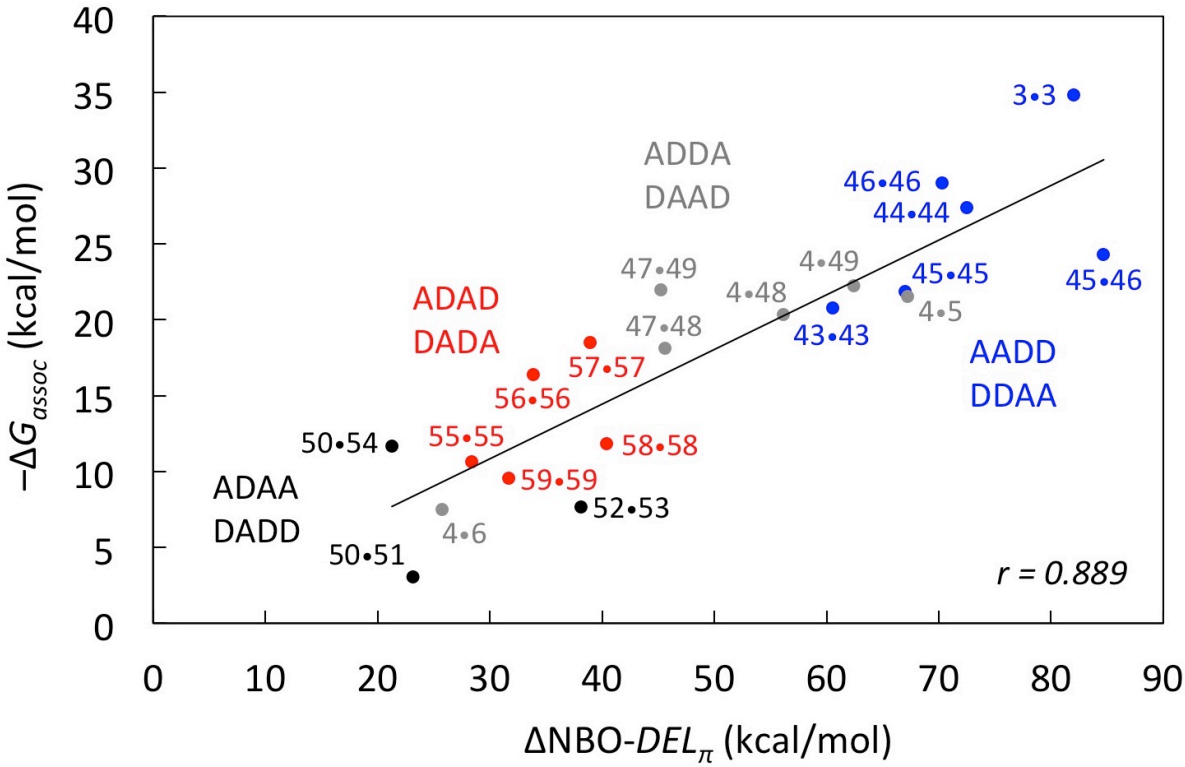

Figure S8. Plot of $-\Delta G_{assoc}$ vs. ΔNBO-DEL_{π} for quadruply hydrogen-bonded arrays in the gas-phase. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. NBO deletion computations were performed at ωB97X-D/def2-TZVPP.

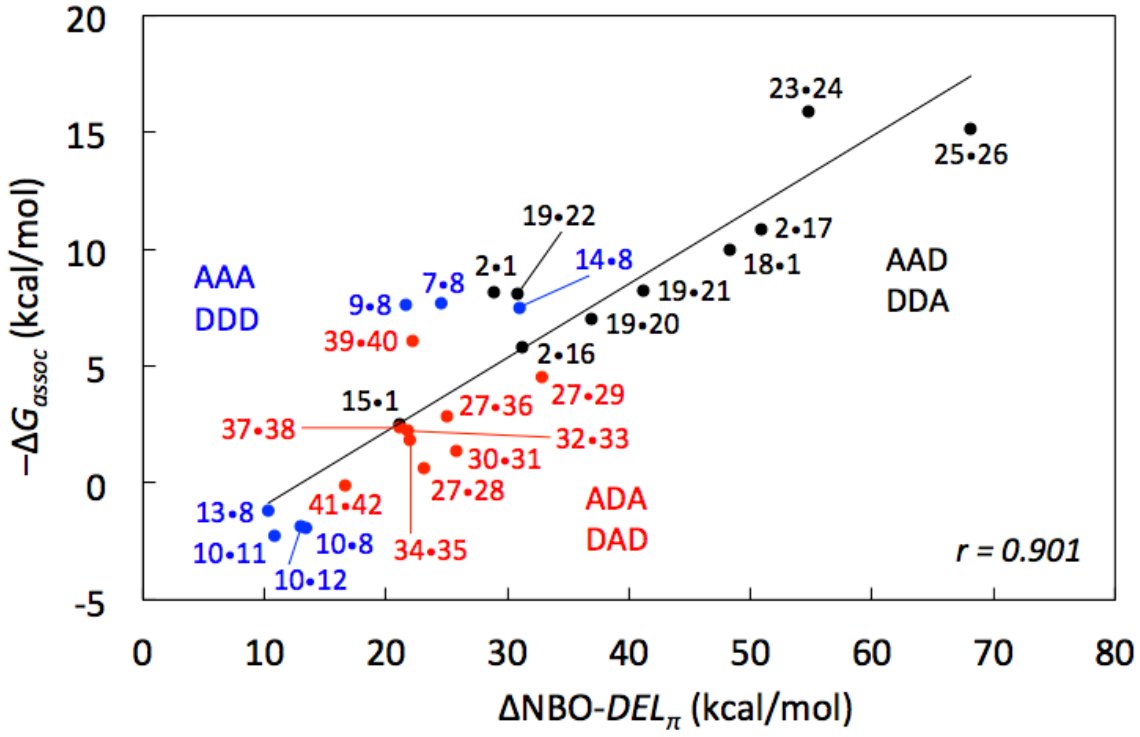

Figure S9. Plot of $-\Delta G_{\text{assoc}}$ vs. ΔNBO-DEL_π for triply hydrogen-bonded arrays in implicit chloroform solvation. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. NBO deletion computations were performed at ωB97X-D/def2-TZVPP.

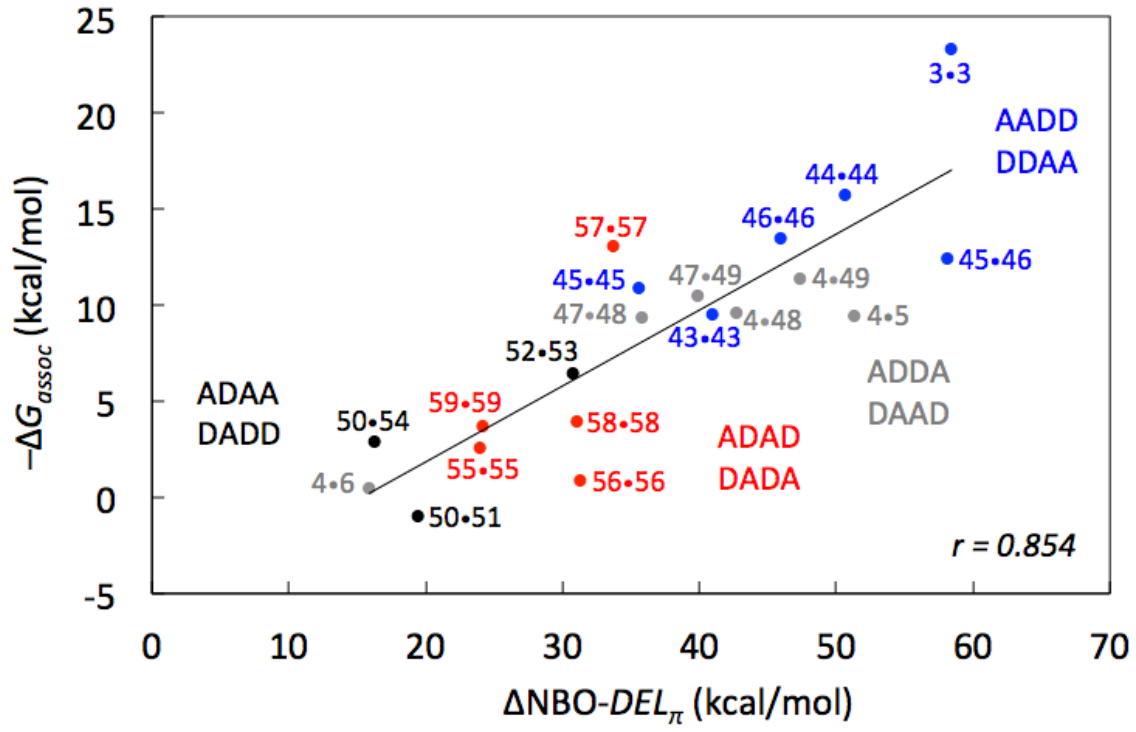

Figure S10. Plot of $-\Delta G_{assoc}$ vs. ΔNBO-DEL_π for triply hydrogen-bonded arrays in implicit chloroform solvation. All geometries were optimized with C_s symmetry at the ωB97X-D/6-311+G(d,p) level. NBO deletion computations were performed at ωB97X-D/def2-TZVPP.

Table S1. Computed DE_{π}, ΔDE_{π}, and $-\Delta G_{\text{assoc}}$ values for triply hydrogen-bonded complexes (A•B) and their monomers (A and B) in the gas-phase. All structures were optimized with C_s symmetry. BLW computations were performed at the B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(\text{A•B})} - [DE_{\pi(\text{A})} + DE_{\pi(\text{B})}]$. Negative values of the association free energies ($-\Delta G_{\text{assoc}}$) were computed at ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DE_{\pi(\text{A•B})}$	$DE_{\pi(\text{A})}$	$DE_{\pi(\text{B})}$	ΔDE_{π}	$-\Delta G_{assoc}$
	7•8	431.95	199.36	218.48	14.11	11.07
	9•8	578.89	364.08	199.36	15.45	11.55
AAA	**10•11**	227.32	99.17	121.66	6.49	2.17
DDD	**10•8**	306.43	99.17	199.36	7.89	0.63
	10•12	353.78	99.17	245.73	8.88	5.32
	13•8	336.09	131.58	199.36	5.15	1.43
	14•8	374.16	156.76	199.36	18.04	11.07
	2•1	346.83	120.36	198.11	28.37	16.51
	15•1	369.74	153.01	198.11	18.62	9.56
	2•16	247.96	120.36	107.16	20.45	11.68
	2•17	292.83	120.36	141.39	31.08	17.72
AAD	**18•1**	342.60	114.09	198.11	30.39	17.76
DDA	**19•20**	345.41	202.37	119.07	23.97	14.44
	19•21	365.87	202.38	139.29	24.21	16.84
	19•22	430.86	202.37	209.58	18.91	16.71
	23•24	373.02	172.01	166.93	34.09	23.48
	25•26	409.38	245.39	119.73	44.26	25.47
	27•28	345.74	107.72	224.44	13.58	4.39
	27•29	397.27	107.72	269.30	20.25	9.29
	30•31	376.69	127.30	235.85	13.54	3.66
	32•33	354.87	118.65	224.52	11.70	6.88
ADA	**34•35**	328.94	124.82	192.06	12.06	6.80
DAD	**27•36**	341.81	219.91	107.73	14.17	5.85
	37•38	384.75	174.75	196.95	13.05	6.19
	39•40	376.78	202.76	163.44	10.58	8.14
	41•42	438.18	159.31	268.65	10.22	3.93

Table S2. Computed NBO-DEL_{π}, ΔNBO-DEL_{π}, and $-\Delta G_{assoc}$ values for triply hydrogen-bonded complexes (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 association free energies ($-\Delta G_{assoc}$) were computed at ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DEL_{\pi(A\bullet B)}$	$DEL_{\pi(A)}$	$DEL_{\pi(B)}$	ΔDEL_{π}	$-\Delta G_{assoc}$
	7•8	707.63	322.78	358.99	25.87	11.07
	9•8	923.73	537.39	358.99	27.35	11.55
	10•11	421.42	185.71	222.77	12.94	2.17
AAA DDD	**10•8**	559.17	185.71	358.99	14.47	0.63
	10•12	643.91	185.71	439.56	18.64	5.32
	13•8	607.16	238.37	358.99	9.80	1.43
	14•8	656.58	265.20	358.99	32.39	11.07
	2•1	608.90	215.00	341.07	52.83	16.51
	15•1	600.68	232.89	341.07	26.73	9.56
	2•16	440.53	215.00	189.35	36.18	11.68
	2•17	531.97	215.00	258.54	58.43	17.72
AAD DDA	**18•1**	600.42	203.35	341.07	56.01	17.76
	19•20	566.57	316.08	207.11	43.38	14.44
	19•21	608.59	316.08	244.93	47.58	16.84
	19•22	696.79	316.08	344.68	36.03	16.71
	23•24	613.52	259.70	289.32	64.50	23.48
	25•26	692.71	394.49	217.76	80.46	25.47
	27•28	605.20	205.98	372.21	27.02	4.39
	27•29	678.47	205.98	434.77	37.72	9.29
	30•31	628.02	225.02	375.80	27.20	3.66
	32•33	603.00	211.04	367.81	24.15	6.88
ADA DAD	**34•35**	560.43	217.51	318.35	24.57	6.80
	27•36	595.46	205.98	361.48	27.99	5.85
	37•38	623.02	278.28	321.25	23.50	6.19
	39•40	607.69	320.05	263.38	24.26	8.14
	41•42	712.06	421.42	267.05	23.59	3.93

Table S3. Computed DE_{π}, ΔDE_{π}, and $-\Delta G_{assoc}$ values for quadruply hydrogen-bonded complexes (A•B) and their monomers (A and B) in the gas-phase. All structures were optimized with C_s symmetry. BLW computations were performed at the B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(A\bullet B)} - [DE_{\pi(A)} + DE_{\pi(B)}]$. Negative values of the association free energies ($-\Delta G_{assoc}$) were computed at ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DE_{\pi(A\bullet B)}$	$DE_{\pi(A)}$	$DE_{\pi(B)}$	ΔDE_{π}	$-\Delta G_{assoc}$
	3•3	394.05	172.94	172.94	46.17	34.80
	43•43	363.67	165.62	165.62	32.43	20.77
AADD	**44•44**	439.85	199.77	199.77	40.31	27.39
DDAA	**45•45**	523.28	246.86	246.86	29.55	21.89
	46•46	539.88	249.53	249.53	40.82	29.00
	45•46	535.83	246.86	249.53	39.43	24.31
	4•5	484.09	203.04	253.90	27.15	21.54
	4•6	487.06	203.04	272.38	11.64	7.49
ADDA	**47•48**	449.40	252.37	174.29	22.74	18.13
DAAD	**47•49**	449.86	246.86	172.50	30.50	21.98
	4•48	404.81	203.04	174.29	27.48	20.35
	4•49	406.21	203.04	172.50	30.67	22.24
	50•51	343.26	183.89	147.20	12.17	3.06
ADAA	**52•53**	454.41	183.89	259.44	11.08	7.66
DADD	**50•54**	404.91	214.39	171.86	18.66	11.67
	55•55	424.62	203.95	203.95	16.72	10.67
	56•56	480.44	231.11	231.11	18.22	16.37
ADAD	**57•57**	426.88	202.75	202.75	21.39	18.50
DADA	**58•58**	451.77	215.73	215.73	20.31	11.81
	59•59	378.77	181.42	181.42	15.94	9.57

Table S4. Computed NBO-DEL_{π}, ΔNBO-DEL_{π}, and $-\Delta G_{assoc}$ values for quadruply hydrogen-bonded complexes (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 association free energies ($-\Delta G_{assoc}$) were computed at ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DEL_{\pi(A\bullet B)}$	$DEL_{\pi(A)}$	$DEL_{\pi(B)}$	ΔDEL_{π}	$-\Delta G_{assoc}$
	3•3	702.60	310.31	310.31	81.98	34.80
	43•43	670.33	304.89	304.89	60.54	20.77
AADD	**44•44**	795.27	361.39	361.39	72.48	27.39
DDAA	**45•45**	914.47	423.76	423.76	66.96	21.89
	46•46	927.91	428.81	428.81	70.30	29.00
	45•46	937.25	423.76	428.81	84.69	24.31
	4•5	810.19	319.73	423.22	67.24	21.54
	4•6	780.76	319.73	435.27	25.75	7.49
ADDA	**47•48**	766.81	411.10	310.09	45.62	18.13
DAAD	**47•49**	758.12	411.10	301.75	45.26	21.98
	4•48	685.96	319.73	310.09	56.15	20.35
	4•49	683.90	319.73	301.75	62.42	22.24
	50•51	600.03	311.31	265.56	23.15	3.06
ADAA	**52•53**	708.66	361.06	309.48	38.12	7.66
DADD	**50•54**	764.15	311.31	431.55	21.28	11.67
	55•55	692.17	331.89	331.89	28.39	10.67
	56•56	816.26	391.19	391.19	33.87	16.37
ADAD	**57•57**	724.68	342.87	342.87	38.94	18.50
DADA	**58•58**	766.79	363.18	363.18	40.42	11.81
	59•59	652.01	310.16	310.16	31.69	9.57

Table S5. Computed DE_{π}, ΔDE_{π}, and $-\Delta G_{\text{assoc}}$ values for triply hydrogen-bonded complexes (A•B) and their monomers (A and B) in implicit chloroform solvation. All structures were optimized with C_s symmetry. BLW computations were performed in implicit chloroform solvation at the PCM-B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(\text{A•B})} - [DE_{\pi(\text{A})} + DE_{\pi(\text{B})}]$. Negative values of the association free energies ($-\Delta G_{\text{assoc}}$) were computed in implicit chloroform solvation at IEF-PCM-ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DE_{\pi(\text{A•B})}$	$DE_{\pi(\text{A})}$	$DE_{\pi(\text{B})}$	ΔDE_{π}	$-\Delta G_{assoc}$
	7•8	439.75	205.85	219.55	14.35	7.68
	9•8	584.72	205.85	364.82	14.05	7.61
AAA	**10•11**	243.64	134.59	103.36	5.70	–2.22
DDD	**10•8**	316.30	103.36	205.85	7.09	–1.89
	10•12	369.88	103.36	258.41	8.11	–1.88
	13•8	344.92	133.93	205.85	5.14	–1.17
	14•8	390.61	167.54	205.85	17.22	7.47
	2•1	353.24	127.56	206.02	19.66	8.19
	15•1	356.26	141.38	206.02	8.86	2.51
	2•16	251.80	127.56	109.25	14.98	5.81
	2•17	307.89	127.56	155.62	24.70	10.86
AAD	**18•1**	347.87	119.42	205.99	22.46	9.96
DDA	**19•20**	347.44	203.44	126.35	17.66	7.03
	19•21	367.23	203.41	145.35	18.47	8.21
	19•22	434.21	203.41	217.02	13.78	8.10
	23•24	371.58	171.96	174.72	24.89	15.92
	25•26	411.94	254.05	126.70	31.18	15.18
	27•28	350.29	112.66	226.98	10.65	0.66
	27•29	407.63	112.66	279.26	15.71	4.57
	30•31	380.28	131.61	238.01	10.66	1.36
	32•33	359.71	123.11	226.14	10.46	2.26
ADA	**34•35**	333.93	129.01	194.33	10.59	1.83
DAD	**27•36**	346.82	221.85	112.66	12.31	2.86
	37•38	389.24	176.27	202.15	10.82	2.37
	39•40	380.66	206.75	164.39	9.51	6.06
	41•42	438.45	269.00	161.28	8.17	–0.09

Table S6. Computed DEL_{π}, ΔDEL_{π}, and $-\Delta G_{\text{assoc}}$ values for triply hydrogen-bonded complexes (A•B) and their monomers (A and B) in implicit chloroform solvation. All structures were optimized with C_s symmetry. NBO deletion computations were performed at the ωB97X-D/def2-TZVPP level; $\Delta DEL_{\pi} = DEL_{\pi(\text{A•B})} - [DEL_{\pi(\text{A})} + DEL_{\pi(\text{B})}]$. Negative values of the association free energies ($-\Delta G_{\text{assoc}}$) were computed in implicit chloroform solvation at IEF-PCM-ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DEL_{\pi(\text{A•B})}$	$DEL_{\pi(\text{A})}$	$DEL_{\pi(\text{B})}$	ΔDEL_{π}	$-\Delta G_{assoc}$
	7•8	714.71	324.19	365.93	24.58	7.68
	9•8	925.34	537.79	365.93	21.62	7.61
	10•11	437.87	190.19	236.82	10.86	–2.22
AAA	**10•8**	569.55	190.19	365.93	13.43	–1.89
DDD	**10•12**	656.59	190.19	453.44	12.97	–1.88
	13•8	617.23	240.99	365.93	10.31	–1.17
	14•8	670.52	273.61	365.93	30.98	7.47
	2•1	600.28	222.18	349.21	28.89	8.19
	15•1	604.30	233.99	349.21	21.10	2.51
	2•16	444.43	222.18	191.11	31.14	5.81
	2•17	542.44	222.18	269.36	50.90	10.86
AAD	**18•1**	606.06	208.58	349.21	48.28	9.96
DDA	**19•20**	567.83	317.55	213.33	36.95	7.03
	19•21	609.74	317.55	251.08	41.11	8.21
	19•22	700.14	317.55	351.77	30.82	8.10
	23•24	612.06	260.02	297.31	54.73	15.92
	25•26	694.02	401.63	224.27	68.12	15.18
	27•28	610.32	211.49	375.67	23.16	0.66
	27•29	685.80	211.49	441.49	32.82	4.57
	30•31	632.68	229.87	377.04	25.78	1.36
	32•33	597.99	216.23	359.98	21.78	2.26
ADA	**34•35**	565.20	222.27	320.94	21.99	1.83
DAD	**27•36**	600.61	211.49	364.11	25.01	2.86
	37•38	627.25	279.04	327.10	21.11	2.37
	39•40	605.71	318.89	264.65	22.18	6.06
	41•42	708.75	422.37	269.76	16.62	–0.09

Table S7. Computed DE_{π}, ΔDE_{π}, and $-\Delta G_{\text{assoc}}$ values for quadruply hydrogen-bonded complexes (A•B) and their monomers (A and B) in implicit chloroform solvation. All structures were optimized with C_s symmetry. BLW computations were performed in implicit chloroform solvation at the PCM-B3LYP/6-31G(d) level; $\Delta DE_{\pi} = DE_{\pi(\text{A•B})} - [DE_{\pi(\text{A})} + DE_{\pi(\text{B})}]$. Negative values of the association free energies ($-\Delta G_{\text{assoc}}$) were computed in implicit chloroform solvation at IEF-PCM-ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DE_{\pi(\text{A•B})}$	$DE_{\pi(\text{A})}$	$DE_{\pi(\text{B})}$	ΔDE_{π}	$-\Delta G_{assoc}$
	3•3	395.38	177.14	177.14	41.10	23.28
	43•43	366.61	168.94	168.94	28.73	9.49
AADD	**44•44**	445.95	204.80	204.80	36.35	15.71
DDAA	**45•45**	513.93	249.17	249.17	15.59	10.87
	46•46	540.94	252.66	252.66	35.62	13.47
	45•46	537.67	249.17	252.66	35.84	12.39
	4•5	474.42	203.47	248.02	22.93	9.39
	4•6	495.29	203.47	277.25	14.57	0.45
ADDA	**47•48**	451.42	253.31	176.57	21.54	9.36
DAAD	**47•49**	451.80	253.31	174.68	23.81	10.50
	4•48	405.06	203.47	176.57	25.02	9.61
	4•49	406.54	203.47	174.68	28.39	11.35
	50•51	346.67	184.57	149.94	12.16	–0.95
ADAA	**52•53**	411.22	217.40	175.34	18.48	6.47
DADD	**50•54**	456.16	184.57	260.78	10.81	2.89
	55•55	403.87	195.48	195.48	12.91	2.61
	56•56	481.91	232.07	232.07	17.77	0.90
ADAD	**57•57**	429.85	206.00	206.00	17.85	13.04
DADA	**58•58**	452.67	216.78	216.78	19.11	3.95
	59•59	379.53	182.19	182.19	15.15	3.67

Table S8. Computed DEL_{π}, ΔDEL_{π}, and $-\Delta G_{\text{assoc}}$ values for quadruply hydrogen-bonded complexes (A•B) and their monomers (A and B) in implicit chloroform solvation. All structures were optimized with C_s symmetry. NBO deletion computations were performed at the ωB97X-D/def2-TZVPP level; $\Delta DEL_{\pi} = DEL_{\pi(\text{A•B})} - [DEL_{\pi(\text{A})} + DEL_{\pi(\text{B})}]$. Negative values of the association free energies ($-\Delta G_{\text{assoc}}$) were computed in implicit chloroform solvation at IEF-PCM-ωB97X-D/6-311+G(d,p). All values are in kcal/mol.

SEI pattern	A•B	$DEL_{\pi(\text{A•B})}$	$DEL_{\pi(\text{A})}$	$DEL_{\pi(\text{B})}$	ΔDEL_{π}	$-\Delta G_{assoc}$
	3•3	709.85	325.72	325.72	58.42	23.28
	43•43	681.31	320.17	320.17	40.98	9.49
AADD DDAA	**44•44**	821.08	385.22	385.22	50.64	15.71
	45•45	905.53	434.98	434.98	35.57	10.87
	46•46	931.68	442.86	442.86	45.97	13.47
	45•46	935.95	434.98	442.86	58.11	12.39
	4•5	806.87	323.90	431.69	51.27	9.39
	4•6	776.99	323.90	437.19	15.90	0.45
ADDA DAAD	**47•48**	772.12	415.71	320.56	35.84	9.36
	47•49	768.77	415.71	313.14	39.92	10.50
	4•48	687.19	323.90	320.56	42.73	9.61
	4•49	684.39	323.90	313.14	47.35	11.35
	50•51	614.97	317.81	277.69	19.47	–0.95
ADAA DADD	**52•53**	734.45	379.29	324.39	30.78	6.47
	50•54	772.07	317.81	437.98	16.27	2.89
	55•55	696.19	336.11	336.11	23.96	2.61
	56•56	825.71	397.21	397.21	31.29	0.90
ADAD DADA	**57•57**	725.63	345.96	345.96	33.71	13.04
	58•58	768.18	368.57	368.57	31.05	3.95
	59•59	651.76	313.80	313.80	24.16	3.67

Table S9. Computed gas-phase planarization energies and planarization free energies (i.e., differences between C_1 minima and fully planar C_s structures) at ωB97X-D/6-31+G(d) for monomers with a nonplanar minima. All values are in kcal/mol.

	ΔE(0K)	ΔG(298K)
1	–0.03	0.05
2	–0.22	0.12
3	0.17	0.44
4	0.36	0.23
8	0.66	1.64
11	2.24	2.57
15	–0.31	–0.14
20	–0.36	–0.37
22	–0.11	–0.48
26	–0.32	–0.14
28	–0.53	–0.18
31	–0.54	–0.44
36	–0.31	–0.20
38	–0.25	–0.14
42	–0.23	0.05
43	–0.34	–0.23
44	–0.03	0.02
45	–0.33	–0.15
46	–0.33	–0.14
50	–0.17	–0.02
51	0.01	1.29
52	0.21	0.31

Table S10. Optimized Cartesian coordinates (in Å) and computed total electronic energies (including thermal free energy corrections) (in a.u.) for all monomers and complexes at ωB97XD/6-311+G(*d*,*p*) in the gas-phase. All the geometries were optimized at C_s symmetry.

1. Triply hydrogen-bonded complexes

AAA–DDD arrays

7•8

	X	Y	Z
C	4.120098	5.003764	0.000000
C	2.891697	4.269381	0.000000
N	2.842717	2.937674	0.000000
C	3.990283	2.260227	0.000000
C	5.271474	2.898063	0.000000
C	5.310531	4.287050	0.000000
N	1.684815	4.912932	0.000000
N	3.880754	0.896876	0.000000
C	6.435012	2.075794	0.000000
H	6.263545	4.808148	0.000000
N	0.004418	1.385677	0.000000
C	–1.156041	2.133153	0.000000
C	0.007437	0.005324	0.000000
N	–0.971546	3.464178	0.000000
C	–2.388378	1.513703	0.000000
C	–2.517326	0.006810	0.000000
C	–1.179117	–0.697854	0.000000
N	1.227564	–0.557666	0.000000
H	2.075716	–0.002572	0.000000
H	–0.046505	3.878655	0.000000
H	–1.816245	4.024280	0.000000
H	1.243244	–1.571069	0.000000
C	4.055778	6.427074	0.000000
C	1.674129	6.214490	0.000000
C	2.841037	7.032489	0.000000
C	4.970738	0.185466	0.000000
C	6.289137	0.726408	0.000000
H	7.415008	2.541320	0.000000
H	7.141156	0.058884	0.000000
H	4.976568	7.000878	0.000000
H	2.738874	8.110027	0.000000
H	0.895916	1.873142	0.000000
C	–3.563656	2.326883	0.000000
C	–1.128779	–2.126143	0.000000
O	–4.715605	1.606809	0.000000
O	–3.633422	3.557471	0.000000
H	–5.424953	2.257652	0.000000
O	–2.356664	–2.707342	0.000000
O	–0.130424	–2.848986	0.000000
H	–2.191546	–3.655766	0.000000

H	4.839339	–0.893980	0.000000
H	0.694458	6.686415	0.000000
H	–3.102913	–0.313385	0.869230
H	–3.102913	–0.313385	–0.869230

Sum of electronic and thermal free energy: –1324.668750 a.u.
N_{Im}= 1 (15*i* cm^{-1})

9•8

	X	Y	Z
C	4.137415	5.021376	0.000000
C	2.921314	4.286902	0.000000
N	2.878436	2.957195	0.000000
C	4.021026	2.275693	0.000000
C	5.295655	2.903128	0.000000
C	5.319307	4.291843	0.000000
N	1.688022	4.909062	0.000000
N	3.879241	0.901652	0.000000
C	6.484102	2.067019	0.000000
H	6.268981	4.811117	0.000000
N	0.020495	1.394478	0.000000
C	–1.140098	2.141672	0.000000
C	0.023208	0.014165	0.000000
N	–0.955645	3.472145	0.000000
C	–2.372845	1.522064	0.000000
C	–2.501925	0.015236	0.000000
C	–1.163698	–0.689277	0.000000
N	1.242848	–0.548563	0.000000
H	2.090339	0.008747	0.000000
H	–0.029095	3.884868	0.000000
H	–1.800359	4.032085	0.000000
H	1.258382	–1.561890	0.000000
C	4.074881	6.473125	0.000000
C	1.646950	6.197025	0.000000
C	2.797723	7.061014	0.000000
C	4.941383	0.172001	0.000000
C	6.289791	0.674544	0.000000
C	7.800213	2.558807	0.000000
C	7.388459	–0.200689	0.000000
C	5.199169	7.315727	0.000000
C	2.653799	8.458293	0.000000
H	0.912252	1.882086	0.000000
C	–3.547678	2.335147	0.000000
C	–1.113194	–2.117137	0.000000
O	–4.700092	1.615181	0.000000
O	–3.618056	3.565935	0.000000
H	–5.408880	2.266586	0.000000
O	–2.341236	–2.698794	0.000000
O	–0.114997	–2.840597	0.000000
H	–2.175336	–3.647048	0.000000
H	4.794334	–0.907581	0.000000

H	0.658717	6.655844	0.000000
H	–3.087532	–0.304970	0.869247
H	–3.087532	–0.304970	–0.869247
H	7.213112	–1.271266	0.000000
C	8.669332	0.301280	0.000000
C	8.869675	1.688960	0.000000
H	7.990619	3.624909	0.000000
H	9.879195	2.083753	0.000000
H	9.520575	–0.368714	0.000000
C	5.044018	8.685512	0.000000
H	1.657875	8.888428	0.000000
C	3.767643	9.265735	0.000000
H	6.199452	6.900684	0.000000
H	5.921192	9.322347	0.000000
H	3.662978	10.343952	0.000000

Sum of electronic and thermal free energy: –1631.841580 a.u.
N_{Im}= 1 (12*i* cm^{-1})

10•11

	X	Y	Z
N	1.216231	1.988412	0.000000
C	–0.008232	1.361446	0.000000
O	0.041385	0.006735	0.000000
C	1.212599	–0.777239	0.000000
C	2.449933	–0.029818	0.000000
C	2.407086	1.309883	0.000000
O	–1.055289	1.938141	0.000000
O	1.063321	–1.959545	0.000000
H	3.296849	1.925849	0.000000
N	–2.825068	–1.539738	0.000000
C	–3.991513	–0.804727	0.000000
C	–2.843083	–2.918482	0.000000
N	–3.821395	0.554125	0.000000
C	–5.195824	–1.432899	0.000000
C	–5.296976	–2.883008	0.000000
C	–4.025514	–3.587209	0.000000
N	–1.610396	–3.514138	0.000000
H	–0.748625	–2.993393	0.000000
H	–2.916136	0.994911	0.000000
H	–4.634948	1.138973	0.000000
H	–1.560811	–4.514881	0.000000
H	–1.938828	–1.059227	0.000000
H	–4.038310	–4.669732	0.000000
H	–6.111127	–0.854720	0.000000
O	–6.380657	–3.471414	0.000000
H	3.377244	–0.580603	0.000000
H	1.187866	2.996188	0.000000
N	1.216231	1.988412	0.000000
C	–0.008232	1.361446	0.000000
O	0.041385	0.006735	0.000000

C	1.212599	–0.777239	0.000000
C	2.449933	–0.029818	0.000000
C	2.407086	1.309883	0.000000
O	–1.055289	1.938141	0.000000
O	1.063321	–1.959545	0.000000
H	3.296849	1.925849	0.000000
N	–2.825068	–1.539738	0.000000
C	–3.991513	–0.804727	0.000000
C	–2.843083	–2.918482	0.000000
N	–3.821395	0.554125	0.000000
C	–5.195824	–1.432899	0.000000
C	–5.296976	–2.883008	0.000000
C	–4.025514	–3.587209	0.000000
N	–1.610396	–3.514138	0.000000

Sum of electronic and thermal free energy: –868.718166 a.u.
N_{Im}= 2 (313*i* cm^{-1}, 308*i* cm^{-1})

10•8

	X	Y	Z
N	4.054901	4.925836	0.000000
C	2.831776	4.296807	0.000000
O	2.883527	2.941928	0.000000
C	4.056469	2.159884	0.000000
C	5.292336	2.909564	0.000000
C	5.246915	4.249216	0.000000
O	1.783230	4.870536	0.000000
O	3.907983	0.977641	0.000000
H	6.135584	4.866749	0.000000
N	0.007321	1.389306	0.000000
C	–1.151696	2.143614	0.000000
C	0.012657	0.006093	0.000000
N	–0.963632	3.476704	0.000000
C	–2.380052	1.524851	0.000000
C	–2.509717	0.017960	0.000000
C	–1.173332	–0.690254	0.000000
N	1.235044	–0.557530	0.000000
H	2.083230	–0.013304	0.000000
H	–0.046987	3.895369	0.000000
H	–1.803875	4.044140	0.000000
H	1.258290	–1.571032	0.000000
H	0.892980	1.870851	0.000000
C	–3.558180	2.340272	0.000000
C	–1.127224	–2.122438	0.000000
O	–4.706980	1.619698	0.000000
O	–3.621909	3.568865	0.000000
H	–5.420027	2.266819	0.000000
O	–2.355864	–2.696648	0.000000
O	–0.129711	–2.842080	0.000000
H	–2.198929	–3.646695	0.000000
H	–3.095371	–0.301041	0.869277

H	–3.095371	–0.301041	–0.869277
H	4.024539	5.933599	0.000000
H	6.220565	2.360322	0.000000

Sum of electronic and thermal free energy: –1171.818319 a.u.
N_{Im}= 3 (105*i* cm^{-1}, 51*i* cm^{-1}, 5*i* cm^{-1})

10•12

	X	Y	Z
N	1.131329	1.950821	0.000000
C	–0.088923	1.322207	0.000000
O	–0.033887	–0.034601	0.000000
C	1.141411	–0.818910	0.000000
C	2.373585	–0.066507	0.000000
C	2.323864	1.273578	0.000000
O	–1.142678	1.885708	0.000000
O	0.984176	–1.999477	0.000000
H	3.211666	1.892288	0.000000
N	–2.775921	–1.520210	0.000000
C	–3.945160	–0.799125	0.000000
C	–2.808060	–2.893684	0.000000
N	–3.852254	0.555179	0.000000
C	–5.173695	–1.418753	0.000000
C	–5.278245	–2.879048	0.000000
C	–3.996797	–3.586577	0.000000
N	–1.621363	–3.552734	0.000000
H	–0.738175	–3.046923	0.000000
H	–2.947264	1.021101	0.000000
C	–4.956697	1.432792	0.000000
C	–1.486745	–4.957512	0.000000
H	–1.886110	–1.038400	0.000000
O	–0.374657	–5.447155	0.000000
C	–2.747773	–5.673383	0.000000
H	–2.686750	–6.753210	0.000000
C	–3.926900	–5.012295	0.000000
O	–4.761104	2.632556	0.000000
C	–6.243663	0.765458	0.000000
H	–7.116240	1.404494	0.000000
C	–6.331157	–0.583716	0.000000
H	–7.292013	–1.086810	0.000000
H	–4.872116	–5.544186	0.000000
O	–6.353834	–3.462729	0.000000
H	1.100624	2.959092	0.000000
H	3.303318	–0.613331	0.000000

Sum of electronic and thermal free energy: –1247.784375 a.u.
N_{Im}= 0

13•8

	X	Y	Z
N	1.238308	2.032969	0.000000
C	0.021118	1.436344	0.000000

O	–0.000394	0.096262	0.000000
C	1.145260	–0.727489	0.000000
C	2.406215	–0.022900	0.000000
C	2.406809	1.318243	0.000000
N	–1.127857	2.024901	0.000000
O	0.951386	–1.902737	0.000000
H	3.313385	1.908894	0.000000
N	–2.879209	–1.576456	0.000000
C	–4.033819	–0.815918	0.000000
C	–2.881604	–2.959734	0.000000
N	–3.836379	0.515485	0.000000
C	–5.265952	–1.427394	0.000000
C	–5.404209	–2.933508	0.000000
C	–4.071467	–3.648974	0.000000
N	–1.661925	–3.529222	0.000000
H	–0.813985	–2.985210	0.000000
H	–2.913121	0.927687	0.000000
H	–4.676622	1.083438	0.000000
H	–1.642733	–4.542779	0.000000
H	–1.992531	–1.097297	0.000000
C	–6.438116	–0.603971	0.000000
C	–4.032925	–5.081616	0.000000
O	–7.591889	–1.315596	0.000000
O	–6.492754	0.625693	0.000000
H	–8.300639	–0.663749	0.000000
O	–5.264417	–5.649053	0.000000
O	–3.038930	–5.805897	0.000000
H	–5.113136	–6.600044	0.000000
H	–5.991486	–3.249537	0.869262
H	–5.991486	–3.249537	–0.869262
H	1.188697	3.057060	0.000000
H	3.313621	–0.606337	0.000000
C	–1.182093	3.405366	0.000000
H	–2.211212	3.784144	0.000000
O	–0.234063	4.171877	0.000000

Sum of electronic and thermal free energy: –1265.233598 a.u.
N_{Im}= 3 (98*i* cm^{-1}, 37*i* cm^{-1}, 11*i* cm^{-1})

14•8

	X	Y	Z
N	–2.232795	0.219488	0.000000
C	–1.064121	–0.608345	0.000000
N	0.128005	0.032178	0.000000
C	0.180006	1.354454	0.000000
C	–0.986464	2.192833	0.000000
C	–2.205247	1.543839	0.000000
O	–1.235216	–1.808942	0.000000
N	1.426165	1.918075	0.000000
H	–3.154254	2.069321	0.000000
N	2.612644	–1.895454	0.000000

C	2.418518	–3.263233	0.000000
C	3.862494	–1.313251	0.000000
N	1.133073	–3.654702	0.000000
C	3.499370	–4.120020	0.000000
C	4.921220	–3.603333	0.000000
C	4.999644	–2.092991	0.000000
N	3.862572	0.032329	0.000000
H	3.008298	0.574080	0.000000
H	0.364269	–2.998096	0.000000
H	0.973785	–4.655319	0.000000
H	4.776545	0.470842	0.000000
H	1.799379	–1.286645	0.000000
C	3.258456	–5.529334	0.000000
C	6.274422	–1.447019	0.000000
O	4.398823	–6.268880	0.000000
O	2.173461	–6.111582	0.000000
H	4.108219	–7.186683	0.000000
O	7.317811	–2.316408	0.000000
O	6.510468	–0.236969	0.000000
H	8.109064	–1.768053	0.000000
H	5.457979	–4.000170	0.869151
H	5.457979	–4.000170	–0.869151
H	–3.107851	–0.288831	0.000000
C	–0.837917	3.606258	0.000000
H	–1.718153	4.240807	0.000000
C	0.416613	4.124706	0.000000
H	0.598910	5.190837	0.000000
C	1.517775	3.218662	0.000000
H	2.528324	3.620888	0.000000

Sum of electronic and thermal free energy: –1246.326492 a.u.
N_{Im}= 1 (24*i* cm^{-1})

AAD–DDA arrays

1•2

	X	Y	Z
C	0.006156	1.325052	0.000000
N	–0.003217	–0.005852	0.000000
C	1.151134	–0.713407	0.000000
O	1.206140	–1.937633	0.000000
N	2.350145	0.009793	0.000000
C	2.383794	1.366189	0.000000
C	1.237512	2.075049	0.000000
N	–1.164796	1.956014	0.000000
C	–3.627329	–0.751115	0.000000
C	–4.813794	–1.543926	0.000000
C	–4.670878	–2.924929	0.000000
N	–3.545517	–3.663488	0.000000
C	–2.457770	–2.921849	0.000000
N	–2.479578	–1.552427	0.000000

O	–3.518657	0.473352	0.000000
N	–1.244817	–3.503480	0.000000
N	–6.146549	–1.184230	0.000000
C	–6.787649	–2.312361	0.000000
N	–5.947331	–3.407824	0.000000
H	3.363653	1.826753	0.000000
H	1.243317	3.155304	0.000000
H	–1.222512	–4.507032	0.000000
H	–0.375144	–2.971102	0.000000
H	–7.861809	–2.424812	0.000000
H	–2.048039	1.419281	0.000000
H	–1.197692	2.959825	0.000000
H	–1.585069	–1.038634	0.000000
H	3.195223	–0.539339	0.000000
H	–6.203968	–4.380532	0.000000

Sum of electronic and thermal free energy: –937.316619 a.u.
N_{Im}= 0

15•1

	X	Y	Z
C	0.033276	1.336117	0.000000
N	0.057649	–0.012516	0.000000
C	1.255116	–0.573551	0.000000
O	1.242346	–1.923822	0.000000
N	2.443213	–0.002934	0.000000
C	2.410204	1.342304	0.000000
C	1.248937	2.065400	0.000000
N	–1.159301	1.936452	0.000000
C	–3.652799	–0.764814	0.000000
C	–4.841946	–1.555951	0.000000
C	–4.707058	–2.936114	0.000000
N	–3.581993	–3.678863	0.000000
C	–2.495652	–2.942401	0.000000
N	–2.504194	–1.573979	0.000000
O	–3.539108	0.455022	0.000000
N	–1.284899	–3.538846	0.000000
N	–6.172043	–1.189355	0.000000
C	–6.819190	–2.314281	0.000000
N	–5.984493	–3.413802	0.000000
H	3.374740	1.840183	0.000000
H	1.253104	3.147105	0.000000
H	–1.269070	–4.542384	0.000000
H	–0.420812	–3.015121	0.000000
H	–7.893851	–2.421147	0.000000
H	–2.031207	1.392446	0.000000
H	–1.211588	2.939058	0.000000
H	–1.608666	–1.067463	0.000000
H	–6.246502	–4.385195	0.000000
H	2.162977	–2.206767	0.000000

Sum of electronic and thermal free energy: –937.303653 a.u.

N_{Im}= 1 (31*i* cm^{-1})

2•16

	X	Y	Z
C	0.026197	1.389589	0.000000
N	–0.027485	0.063193	0.000000
C	1.109469	–0.682447	0.000000
O	1.124992	–1.902613	0.000000
N	2.328361	0.010017	0.000000
C	2.401466	1.362997	0.000000
C	1.275269	2.105301	0.000000
N	–1.128187	2.060148	0.000000
C	–3.566655	–0.736091	0.000000
C	–4.810002	–1.536590	0.000000
C	–4.703131	–3.012075	0.000000
N	–3.631286	–3.690434	0.000000
C	–2.423131	–2.956158	0.000000
N	–2.465282	–1.536668	0.000000
O	–3.524348	0.481277	0.000000
N	–1.348368	–3.618338	0.000000
N	–6.036260	–1.174023	0.000000
C	–6.726557	–2.437675	0.000000
N	–6.018487	–3.508369	0.000000
H	3.393970	1.795672	0.000000
H	1.311504	3.184849	0.000000
H	–0.510485	–3.023902	0.000000
H	–7.809264	–2.436795	0.000000
H	–2.013332	1.547969	0.000000
H	–1.136235	3.064044	0.000000
H	–1.559150	–1.034347	0.000000
H	3.157266	–0.563900	0.000000

Sum of electronic and thermal free energy: –936.024917 a.u.
N_{Im}= 0

2•17

	X	Y	Z
C	0.023455	1.369095	0.000000
N	–0.032079	0.039662	0.000000
C	1.101364	–0.703664	0.000000
O	1.112159	–1.929832	0.000000
N	2.319992	–0.022724	0.000000
C	2.398496	1.331388	0.000000
C	1.275490	2.077730	0.000000
N	–1.127365	2.041053	0.000000
C	–3.604303	–0.725289	0.000000
C	–4.844793	–1.542092	0.000000
C	–4.734128	–3.045972	0.000000
N	–3.550661	–3.677835	0.000000
C	–2.483897	–2.905973	0.000000
N	–2.479672	–1.512558	0.000000

O	–3.553237	0.486377	0.000000
N	–1.278970	–3.464065	0.000000
N	–6.047082	–1.155974	0.000000
C	–6.793391	–2.463760	0.000000
N	–5.918139	–3.564241	0.000000
H	3.392833	1.759254	0.000000
H	1.316537	3.157055	0.000000
H	–1.254968	–4.470313	0.000000
H	–0.406886	–2.925260	0.000000
O	–7.982429	–2.484098	0.000000
H	–2.016539	1.536289	0.000000
H	–1.133305	3.045389	0.000000
H	–1.575864	–1.004893	0.000000
H	3.147243	–0.599291	0.000000

Sum of electronic and thermal free energy: –1011.304441 a.u.
N_{Im}= 0

18•1

	X	Y	Z
O	0.080666	–1.770619	0.000000
C	1.235977	–1.332235	0.000000
N	1.450666	0.043128	0.000000
C	2.667436	0.667946	0.000000
N	3.811445	0.018568	0.000000
C	3.641931	–1.316905	0.000000
C	2.462633	–2.053944	0.000000
N	2.725574	–3.408650	0.000000
C	4.020279	–3.487710	0.000000
N	4.635389	–2.251339	0.000000
N	2.643879	2.013914	0.000000
O	–2.210525	–0.581960	0.000000
C	–2.202506	0.715267	0.000000
N	–1.059655	1.373626	0.000000
C	–1.025287	2.734262	0.000000
N	–2.255027	3.393424	0.000000
C	–3.442390	2.731817	0.000000
C	–3.471766	1.383112	0.000000
O	0.009798	3.386186	0.000000
H	–2.215638	4.400932	0.000000
H	–4.334874	3.344426	0.000000
H	–1.280142	–0.987099	0.000000
H	0.586936	0.608746	0.000000
H	1.774096	2.542638	0.000000
H	3.527601	2.489882	0.000000
H	5.622210	–2.055143	0.000000
H	4.593542	–4.403018	0.000000
H	–4.391317	0.819010	0.000000

Sum of electronic and thermal free energy: –957.197646 a.u.
N_{Im}= 0

19•20

	X	Y	Z
C	–1.738129	1.675724	0.000000
C	–0.368233	1.264158	0.000000
N	0.002057	–0.003126	0.000000
C	–0.952787	–0.962417	0.000000
C	–2.334894	–0.655265	0.000000
C	–2.698211	0.715497	0.000000
N	0.665751	2.176367	0.000000
N	–0.512801	–2.246016	0.000000
C	–3.259108	–1.716005	0.000000
H	–3.748315	0.988969	0.000000
H	–1.969538	2.730030	0.000000
N	2.934578	–0.818632	0.000000
C	3.780050	0.280861	0.000000
C	3.336385	–2.119411	0.000000
O	3.280932	1.421415	0.000000
C	5.183232	0.005168	0.000000
C	5.584050	–1.307344	0.000000
C	4.689989	–2.389931	0.000000
N	2.355772	–3.054581	0.000000
H	1.630429	1.787249	0.000000
C	0.595377	3.545717	0.000000
H	1.607699	3.979514	0.000000
O	–0.404475	4.227068	0.000000
H	–4.322381	–1.498516	0.000000
C	–2.797055	–3.006184	0.000000
H	–3.469846	–3.853975	0.000000
C	–1.405472	–3.211150	0.000000
H	1.930417	–0.601657	0.000000
C	6.126440	1.170926	0.000000
H	6.648946	–1.523761	0.000000
H	5.039448	–3.413180	0.000000
H	7.164006	0.829412	0.000000
H	5.969062	1.804922	0.877337
H	5.969062	1.804922	–0.877337
H	1.369719	–2.790795	0.000000
H	–1.012887	–4.225157	0.000000
H	2.612150	–4.023605	0.000000

Sum of electronic and thermal free energy: –1004.597353 a.u.
N_{Im}= 1 (100*i* cm^{-1})

19•21

	X	Y	Z
N	1.466274	–3.388705	0.000000
C	0.376450	–4.125856	0.000000
C	–0.930303	–3.608353	0.000000
C	–1.085121	–2.246481	0.000000
C	0.056422	–1.424594	0.000000
C	1.331603	–2.038458	0.000000

N	2.481395	–1.324264	0.000000
C	2.409751	–0.005195	0.000000
C	1.170110	0.708006	0.000000
C	0.015963	–0.007000	0.000000
N	3.623417	0.647775	0.000000
C	3.867079	1.998517	0.000000
O	3.048106	2.887909	0.000000
O	4.662635	–7.036081	0.000000
C	3.816489	–6.174994	0.000000
N	4.015121	–4.823683	0.000000
C	5.239468	–4.166697	0.000000
C	6.476432	–4.747219	0.000000
C	7.602176	–3.891721	0.000000
C	7.512687	–2.528963	0.000000
C	6.204855	–1.930963	0.000000
N	5.135722	–2.804551	0.000000
O	5.994268	–0.706624	0.000000
C	8.694377	–1.608445	0.000000
H	–0.943690	0.499291	0.000000
H	1.186276	1.787295	0.000000
H	4.471301	0.049017	0.000000
H	4.951499	2.190788	0.000000
H	–2.070679	–1.792268	0.000000
H	–1.778662	–4.280150	0.000000
H	4.208579	–2.358651	0.000000
H	8.586740	–4.350094	0.000000
H	6.571071	–5.820130	0.000000
H	9.627764	–2.174546	0.000000
H	8.678982	–0.955475	0.876957
H	8.678982	–0.955475	–0.876957
H	3.160613	–4.248674	0.000000
H	2.737013	–6.409558	0.000000
H	0.525937	–5.202643	0.000000

Sum of electronic and thermal free energy: –1117.662603 a.u.
N_{Im}= 0

19•22

	X	Y	Z
N	0.639617	–2.209743	0.000000
C	0.323529	–3.486064	0.000000
C	–0.994216	–3.977614	0.000000
C	–2.021211	–3.070375	0.000000
C	–1.723442	–1.695311	0.000000
C	–0.364875	–1.297603	0.000000
N	0.008720	0.003689	0.000000
C	–0.927625	0.934355	0.000000
C	–2.325742	0.634287	0.000000
C	–2.703140	–0.670108	0.000000
N	–0.463198	2.233219	0.000000
C	–1.185041	3.400960	0.000000

O	–2.389006	3.512634	0.000000
N	3.534387	–1.558832	0.000000
C	3.952012	–0.278866	0.000000
N	5.236468	–0.002283	0.000000
C	5.479016	1.324035	0.000000
C	4.575400	2.378111	0.000000
C	3.185040	2.065423	0.000000
O	2.222278	2.828683	0.000000
N	2.971557	0.679210	0.000000
N	5.234707	3.588047	0.000000
C	6.492997	3.265490	0.000000
N	6.713281	1.902574	0.000000
H	–3.754837	–0.937213	0.000000
H	–3.037249	1.445931	0.000000
H	4.245031	–2.267645	0.000000
H	2.542362	–1.801520	0.000000
C	7.979997	1.203253	0.000000
H	7.320619	3.961060	0.000000
H	0.564567	2.355137	0.000000
H	–3.057474	–3.392780	0.000000
H	–1.174572	–5.044759	0.000000
H	1.986544	0.386533	0.000000
H	–0.507733	4.269168	0.000000
H	8.784953	1.938099	0.000000
H	1.156712	–4.184645	0.000000
H	8.065393	0.574326	0.887576
H	8.065393	0.574326	–0.887576

Sum of electronic and thermal free energy: –1167.987061 a.u.
N_{Im}= 0

23•24

	X	Y	Z
O	3.555481	1.980650	0.000000
C	2.447876	1.307468	0.000000
C	1.226097	2.068632	0.000000
C	0.041957	1.416980	0.000000
C	0.020664	–0.009471	0.000000
C	1.268268	–0.679464	0.000000
N	2.451033	–0.015428	0.000000
C	–1.151815	–0.777293	0.000000
C	–1.061171	–2.149299	0.000000
C	0.216391	–2.723100	0.000000
N	1.341344	–2.032780	0.000000
N	5.781500	0.728785	0.000000
C	6.037837	–0.547937	0.000000
C	7.350396	–1.167611	0.000000
C	7.429914	–2.523397	0.000000
C	6.283599	–3.366473	0.000000
C	5.050227	–2.747104	0.000000
N	4.955827	–1.393880	0.000000

C	6.385505	–4.827861	0.000000
O	7.460589	–5.417475	0.000000
C	5.094168	–5.512084	0.000000
C	3.935407	–4.821617	0.000000
N	3.890585	–3.453952	0.000000
H	–0.896264	1.962304	0.000000
H	1.301120	3.147911	0.000000
H	2.986831	–2.955408	0.000000
H	–2.116654	–0.280047	0.000000
H	–1.940598	–2.779795	0.000000
C	8.558274	–0.278479	0.000000
H	8.395164	–3.020380	0.000000
H	8.579460	0.368586	–0.883914
H	8.579460	0.368586	0.883914
H	9.471282	–0.874618	0.000000
H	6.618752	1.295527	0.000000
H	2.967946	–5.308280	0.000000
H	5.088528	–6.593812	0.000000
H	0.320264	–3.805098	0.000000
H	4.448840	1.398712	0.000000
H	4.021438	–0.942390	0.000000

Sum of electronic and thermal free energy: –1080.531621 a.u.
N_{Im}= 0

25•26

	X	Y	Z
C	1.221572	2.115525	0.000000
C	0.025906	1.359701	0.000000
N	–0.008578	–0.004632	0.000000
C	1.157750	–0.630964	0.000000
C	2.440073	–0.015680	0.000000
C	2.528524	1.450878	0.000000
N	–1.178493	1.973462	0.000000
N	1.129009	–2.001612	0.000000
C	3.574725	–0.806732	0.000000
O	3.593972	2.050815	0.000000
N	–2.503370	–1.436871	0.000000
C	–3.703259	–0.813467	0.000000
C	–2.420647	–2.820042	0.000000
N	–3.709115	0.518365	0.000000
N	–4.845502	–1.492060	0.000000
C	–4.695069	–2.825269	0.000000
N	–3.589998	–3.529202	0.000000
N	–1.242554	–3.353093	0.000000
H	–2.832713	1.059502	0.000000
H	–5.623010	–3.392904	0.000000
H	–4.608459	0.966978	0.000000
H	–1.340480	–4.362845	0.000000
C	1.133478	3.506931	0.000000
C	–1.243329	3.299747	0.000000

C	–2.623287	3.898118	0.000000
C	–0.102462	4.113712	0.000000
C	2.224977	–2.774092	0.000000
C	1.999543	–4.254460	0.000000
C	3.481946	–2.194206	0.000000
H	–2.589177	4.987945	0.000000
H	–3.176165	3.568718	–0.883897
H	–3.176165	3.568718	0.883897
H	2.949798	–4.786659	0.000000
H	1.425378	–4.551008	0.881021
H	1.425378	–4.551008	–0.881021
H	4.537230	–0.305460	0.000000
H	4.362805	–2.821339	0.000000
H	2.055204	4.078523	0.000000
H	–0.202965	5.191675	0.000000
H	–1.619102	–0.887961	0.000000
H	0.174009	–2.494138	0.000000

Sum of electronic and thermal free energy: –1132.317792 a.u.
N_{Im}= 0

ADA–DAD arrays

27•28

	X	Y	Z
O	6.099160	0.389761	0.000000
C	6.096817	–0.829248	0.000000
C	7.300614	–1.646571	0.000000
C	7.189458	–2.983337	0.000000
N	5.964633	–3.596538	0.000000
C	4.768086	–2.901949	0.000000
N	4.899249	–1.538203	0.000000
O	3.701077	–3.484640	0.000000
N	3.669704	1.961721	0.000000
C	2.482809	1.341751	0.000000
N	2.421110	0.001056	0.000000
C	1.198980	–0.597902	0.000000
N	0.003472	0.000804	0.000000
C	0.111060	1.327472	0.000000
C	1.278207	2.071689	0.000000
N	1.193532	–1.949234	0.000000
N	1.014402	3.429264	0.000000
C	–0.283222	3.499548	0.000000
N	–0.892144	2.260730	0.000000
H	8.045407	–3.646136	0.000000
H	8.257841	–1.148540	0.000000
H	4.008941	–0.987878	0.000000
H	0.301337	–2.408087	0.000000
H	2.047320	–2.492662	0.000000
H	3.679250	2.966915	0.000000
H	4.544558	1.443789	0.000000

H	–0.861069	4.411994	0.000000
H	5.879283	–4.600164	0.000000
H	–1.878763	2.065245	0.000000

Sum of electronic and thermal free energy: –937.322268 a.u.
N_{Im}= 1 (29*i* cm^{-1})

27•29

	X	Y	Z
O	–3.726440	0.222223	0.000000
C	–3.494966	1.416143	0.000000
C	–4.510801	2.458628	0.000000
C	–4.134790	3.745786	0.000000
N	–2.809466	4.104673	0.000000
C	–1.784804	3.185099	0.000000
N	–2.179294	1.880630	0.000000
O	–0.613733	3.540529	0.000000
N	–1.541107	–1.754513	0.000000
C	–0.271925	–1.343217	0.000000
N	–0.009313	–0.014283	0.000000
C	1.274999	0.368590	0.000000
C	2.420633	–0.493465	0.000000
C	2.115629	–1.886996	0.000000
C	0.776562	–2.289637	0.000000
N	1.515111	1.707496	0.000000
H	–4.840319	4.566564	0.000000
H	–5.548861	2.163727	0.000000
H	–1.411129	1.168370	0.000000
H	0.702858	2.340326	0.000000
H	–1.698280	–2.749818	0.000000
H	–2.326010	–1.110570	0.000000
C	3.687002	0.066864	0.000000
C	2.745569	2.252788	0.000000
H	2.778696	3.333726	0.000000
C	3.860091	1.453108	0.000000
H	4.844405	1.900214	0.000000
H	4.539059	–0.603717	0.000000
N	0.711675	–3.645900	0.000000
H	–2.527856	5.071956	0.000000
N	2.908748	–2.971534	0.000000
C	2.006725	–3.980609	0.000000
H	2.324824	–5.015591	0.000000

Sum of electronic and thermal free energy: –1035.527092 a.u.
N_{Im}= 0

30•31

	X	Y	Z
C	7.281210	–1.659022	0.000000
C	6.085576	–0.820371	0.000000
N	4.900597	–1.540543	0.000000
C	4.764605	–2.905396	0.000000

N	5.947868	–3.626546	0.000000
C	7.164091	–2.997863	0.000000
O	6.093313	0.394310	0.000000
O	3.686974	–3.471296	0.000000
C	2.484436	1.349034	0.000000
C	1.280936	2.079309	0.000000
C	0.113477	1.336060	0.000000
N	0.005109	0.007913	0.000000
C	1.199984	–0.590938	0.000000
N	2.423380	0.006845	0.000000
N	3.670503	1.970694	0.000000
N	1.192688	–1.942912	0.000000
N	1.013201	3.434285	0.000000
C	–0.286737	3.493859	0.000000
N	–0.898987	2.257188	0.000000
C	5.838319	–5.082132	0.000000
H	8.033289	–3.642718	0.000000
Cl	8.826992	–0.890650	0.000000
H	4.007975	–0.989887	0.000000
H	6.841271	–5.505966	0.000000
H	5.298056	–5.417583	0.885440
H	5.298056	–5.417583	–0.885440
H	0.299528	–2.399700	0.000000
H	2.045757	–2.486867	0.000000
H	3.677806	2.975963	0.000000
H	4.545830	1.455650	0.000000
C	–2.314747	1.961953	0.000000
H	–0.872667	4.402464	0.000000
H	–2.870201	2.899953	0.000000
H	–2.580578	1.384772	–0.887235
H	–2.580578	1.384772	0.887235

Sum of electronic and thermal free energy: –1475.497204 a.u.
N_{Im}= 1 (32*i* cm^{-1})

32•33

	X	Y	Z
C	1.239553	–0.771928	0.000000
O	1.306362	–1.990056	0.000000
N	2.397855	–0.003201	0.000000
C	2.470411	1.364308	0.000000
O	3.528167	1.972196	0.000000
N	1.258445	2.030615	0.000000
C	0.074387	1.339016	0.000000
C	0.012146	–0.003248	0.000000
N	5.008204	–1.459539	0.000000
C	5.053906	–2.805725	0.000000
C	6.231844	–3.533467	0.000000
C	7.428969	–2.820112	0.000000
C	7.418442	–1.428884	0.000000
C	6.174235	–0.805515	0.000000

O	8.551303	–3.553397	0.000000
N	6.055299	0.586578	0.000000
C	7.045401	1.526628	0.000000
O	8.240590	1.334741	0.000000
N	3.800422	–3.416999	0.000000
C	3.506205	–4.752119	0.000000
O	4.289090	–5.673552	0.000000
C	1.302826	3.489857	0.000000
H	–0.817068	1.953801	0.000000
H	–0.929616	–0.530029	0.000000
H	3.305845	–0.507625	0.000000
H	0.281538	3.867249	0.000000
H	1.826406	3.850258	0.885627
H	1.826406	3.850258	–0.885627
H	5.109799	0.966320	0.000000
H	2.985214	–2.804043	0.000000
C	9.799644	–2.881432	0.000000
H	10.555433	–3.664121	0.000000
H	9.914422	–2.260635	–0.893697
H	9.914422	–2.260635	0.893697
H	2.413637	–4.904470	0.000000
H	6.612887	2.541425	0.000000
H	6.224721	–4.611749	0.000000
H	8.310219	–0.825117	0.000000

Sum of electronic and thermal free energy: –1154.086057 a.u.
N_{Im}= 0

34•35

	X	Y	Z
O	1.311424	–1.981594	0.000000
C	1.252226	–0.760797	0.000000
N	2.411578	–0.002294	0.000000
C	2.493847	1.366202	0.000000
O	3.558621	1.963958	0.000000
N	1.287926	2.030030	0.000000
C	0.096642	1.340382	0.000000
C	0.009466	–0.002265	0.000000
O	4.254541	–5.688617	0.000000
C	3.481473	–4.758627	0.000000
N	3.789574	–3.426596	0.000000
C	5.050222	–2.829918	0.000000
N	5.028878	–1.489759	0.000000
C	6.196865	–0.832944	0.000000
C	7.432271	–1.478664	0.000000
C	7.422619	–2.863375	0.000000
C	6.232241	–3.570026	0.000000
N	6.075088	0.557513	0.000000
C	7.067661	1.497237	0.000000
O	8.260936	1.301871	0.000000
C	1.332213	3.488976	0.000000

H	–0.789399	1.964191	0.000000
C	–1.284266	–0.754899	0.000000
H	3.313582	–0.512088	0.000000
H	0.311167	3.866884	0.000000
H	1.855815	3.849894	0.885574
H	1.855815	3.849894	–0.885574
H	5.130365	0.939885	0.000000
H	2.979704	–2.805472	0.000000
H	2.387482	–4.899614	0.000000
H	6.195395	–4.647804	0.000000
H	8.344399	–0.903368	0.000000
H	6.635447	2.512338	0.000000
H	–2.135251	–0.071354	0.000000
H	–1.353830	–1.401287	–0.878072
H	–1.353830	–1.401287	0.878072
H	8.362962	–3.403064	0.000000

Sum of electronic and thermal free energy: –1078.882105 a.u.
N_{Im}= 0

27•36

	X	Y	Z
O	2.758738	2.995070	0.000000
C	1.955625	2.082911	0.000000
N	2.304329	0.758899	0.000000
C	1.438336	–0.322506	0.000000
O	1.879757	–1.462787	0.000000
N	0.591275	2.311890	0.000000
C	–0.337943	1.305057	0.000000
C	0.025485	0.012483	0.000000
N	5.063391	0.005294	0.000000
C	6.045827	0.948838	0.000000
N	7.359845	0.725022	0.000000
C	7.650126	–0.572770	0.000000
C	6.756919	–1.640899	0.000000
C	5.400603	–1.286212	0.000000
O	4.479191	–2.219877	0.000000
N	5.645295	2.240024	0.000000
N	8.887246	–1.153622	0.000000
C	8.680794	–2.520371	0.000000
N	7.427515	–2.851815	0.000000
H	0.314494	3.280574	0.000000
H	–1.372420	1.624008	0.000000
H	4.670046	2.510723	0.000000
H	6.359332	2.945139	0.000000
H	9.766814	–0.665709	0.000000
H	9.509759	–3.213133	0.000000
H	3.326627	0.533020	0.000000
H	3.564154	–1.858342	0.000000
H	–0.696643	–0.789199	0.000000

Sum of electronic and thermal free energy: –957.196962 a.u.

N_{Im}= 1 (19*i* cm^{-1})

37•38

	X	Y	Z
C	–4.284168	0.765144	0.000000
C	–3.122420	–0.121789	0.000000
N	–1.892034	0.501224	0.000000
C	–1.716251	1.859019	0.000000
C	–2.840919	2.707923	0.000000
C	–4.146211	2.102097	0.000000
O	–3.215093	–1.342510	0.000000
N	–0.459580	2.314546	0.000000
C	–2.610507	4.083290	0.000000
H	–5.017884	2.748816	0.000000
H	–5.250335	0.278279	0.000000
N	0.479967	–1.324342	0.000000
C	0.312567	–2.650569	0.000000
C	1.738405	–0.849944	0.000000
N	–0.954821	–3.116189	0.000000
C	1.407716	–3.573017	0.000000
C	2.667480	–3.043562	0.000000
C	2.878275	–1.654234	0.000000
N	1.881332	0.512959	0.000000
C	3.115686	1.087897	0.000000
H	1.044124	1.100082	0.000000
H	–3.454175	4.765574	0.000000
C	–1.312802	4.558806	0.000000
H	–1.096158	5.618719	0.000000
C	–0.275723	3.629511	0.000000
C	1.152299	–5.053251	0.000000
H	3.545299	–3.682148	0.000000
C	4.233321	–1.082401	0.000000
H	2.094762	–5.601958	0.000000
H	–1.129373	–4.103282	0.000000
H	–1.751923	–2.482775	0.000000
H	–1.053014	–0.111022	0.000000
H	3.113562	2.171625	0.000000
C	4.262389	0.373419	0.000000
O	5.242457	–1.780344	0.000000
H	5.222507	0.871605	0.000000
H	0.757591	3.963209	0.000000
H	0.587266	–5.366992	0.885351
H	0.587266	–5.366992	–0.885351

Sum of electronic and thermal free energy: –1080.797486 a.u.
N_{Im}= 1 (25*i* cm^{-1})

39•40

	X	Y	Z
N	–1.090320	–0.785531	0.000000
C	–2.268147	–0.179813	0.000000

C	–2.430457	1.207649	0.000000
C	–1.299486	1.995970	0.000000
C	–0.039198	1.389182	0.000000
C	0.003106	–0.016066	0.000000
N	1.212548	–0.653863	0.000000
C	2.417326	–0.016548	0.000000
C	2.385990	1.432266	0.000000
C	1.207957	2.091375	0.000000
N	3.471787	–0.805380	0.000000
C	4.766327	–0.323324	0.000000
O	5.148349	0.827921	0.000000
O	–2.579658	–5.412154	0.000000
C	–2.238985	–4.251572	0.000000
N	–0.971649	–3.755233	0.000000
C	0.237882	–4.459413	0.000000
C	0.307024	–5.841961	0.000000
C	1.576576	–6.416731	0.000000
C	2.718647	–5.644698	0.000000
C	2.526058	–4.248976	0.000000
N	1.327228	–3.667382	0.000000
O	3.617799	–3.495960	0.000000
H	1.194731	3.176522	0.000000
H	3.335656	1.943781	0.000000
H	5.489016	–1.155161	0.000000
H	–1.371259	3.078389	0.000000
H	–3.422889	1.638348	0.000000
C	4.107066	–6.212742	0.000000
H	1.666380	–7.498631	0.000000
H	–0.594057	–6.434074	0.000000
H	4.075985	–7.304088	0.000000
H	4.667768	–5.880332	0.877740
H	4.667768	–5.880332	–0.877740
H	–0.903691	–2.737044	0.000000
H	–2.976978	–3.427623	0.000000
H	–3.136924	–0.831323	0.000000
H	1.222608	–1.693210	0.000000
H	3.423035	–2.519088	0.000000

Sum of electronic and thermal free energy: –1117.646027 a.u.
N_{Im}= 1 (3*i* cm^{-1})

41•42

	X	Y	Z
C	–2.389579	–1.470940	0.000000
C	–1.135706	–2.106376	0.000000
N	0.020710	–1.374111	0.000000
C	0.005805	–0.005430	0.000000
C	–1.209615	0.700779	0.000000
C	–2.500683	–0.004158	0.000000
N	–1.000878	–3.438148	0.000000
N	1.196511	0.606138	0.000000

C	–1.146061	2.092746	0.000000
O	–3.572601	0.578249	0.000000
H	0.929220	–1.867734	0.000000
N	2.663839	–2.810209	0.000000
C	2.760223	–4.149077	0.000000
C	3.839580	–2.162527	0.000000
N	1.622895	–4.858192	0.000000
N	3.916742	–4.841183	0.000000
C	4.998264	–4.078577	0.000000
N	5.049569	–2.756220	0.000000
N	3.815639	–0.822457	0.000000
H	2.930052	–0.317963	0.000000
H	0.717737	–4.389717	0.000000
H	5.953971	–4.597843	0.000000
H	1.700158	–5.859479	0.000000
H	4.697749	–0.342428	0.000000
C	–3.522838	–2.281703	0.000000
C	–2.094177	–4.196692	0.000000
C	–1.869144	–5.681833	0.000000
C	–3.384482	–3.653247	0.000000
C	1.237998	1.936164	0.000000
C	2.606464	2.555507	0.000000
C	0.079932	2.722996	0.000000
H	–2.810877	–6.231118	0.000000
H	–1.294471	–5.973465	–0.883007
H	–1.294471	–5.973465	0.883007
H	2.554861	3.644502	0.000000
H	3.163849	2.232055	0.883007
H	3.163849	2.232055	–0.883007
H	–2.078195	2.646739	0.000000
H	0.157461	3.802696	0.000000
H	–4.494853	–1.801111	0.000000
H	–4.248149	–4.305813	0.000000

Sum of electronic and thermal free energy: –1132.343115 a.u.
N_{Im}= 0

2. Quadruply hydrogen-bonded complexes

AADD-DDAA arrays

3•3

	X	Y	Z
O	2.589260	–2.546240	0.000000
C	2.799680	–1.331180	0.000000
C	4.149920	–0.796160	0.000000
C	4.344550	0.537000	0.000000
N	3.245600	1.359260	0.000000
C	1.992690	0.845350	0.000000
N	1.741240	–0.441380	0.000000
N	0.944520	1.719020	0.000000

C	1.054810	3.120040	0.000000
O	2.149490	3.690050	0.000000
N	–0.112540	3.760970	0.000000
H	–1.003690	3.245300	0.000000
H	0.010570	1.280010	0.000000
H	3.290730	2.386610	0.000000
C	5.672270	1.222350	0.000000
H	4.977850	–1.490720	0.000000
O	–2.589270	2.546260	0.000000
C	–2.799690	1.331200	0.000000
C	–4.149910	0.796150	0.000000
C	–4.344520	–0.537020	0.000000
N	–3.245550	–1.359250	0.000000
C	–1.992650	–0.845310	0.000000
N	–1.741230	0.441420	0.000000
N	–0.944480	–1.718960	0.000000
C	–1.054820	–3.119970	0.000000
O	–2.149530	–3.689930	0.000000
N	0.112520	–3.760930	0.000000
H	1.003680	–3.245290	0.000000
H	–0.010530	–1.279970	0.000000
H	–3.290660	–2.386600	0.000000
C	–5.672230	–1.222400	0.000000
H	–4.977850	1.490700	0.000000
C	–0.151910	5.208280	0.000000
C	0.151850	–5.208250	0.000000
H	6.478790	0.490570	0.000000
H	5.774090	1.858480	–0.883500
H	5.774090	1.858480	0.883500
H	–1.197720	5.512970	0.000000
H	0.341300	5.617310	0.885220
H	0.341300	5.617310	–0.885220
H	1.197650	–5.512970	0.000000
H	–0.341370	–5.617270	0.885220
H	–0.341370	–5.617270	–0.885220
H	–6.478760	–0.490630	0.000000
H	–5.774030	–1.858530	–0.883500
H	–5.774030	–1.858530	0.883500

Sum of electronic and thermal free energy: –1284.254092 a.u.
N_{Im}= 0

43•43

	X	Y	Z
O	–3.035950	1.935620	0.000000
C	–1.902430	2.406690	0.000000
N	–1.774010	3.791930	0.000000
C	–0.569050	4.409480	0.000000
C	0.569050	3.686150	0.000000
C	0.422400	2.258440	0.000000
N	–0.765870	1.662430	0.000000

N	1.494490	1.421890	0.000000
C	2.860240	1.799770	0.000000
O	3.228820	2.959730	0.000000
N	3.695490	0.748660	0.000000
H	3.403590	–0.232930	0.000000
H	1.259320	0.424000	0.000000
H	1.544210	4.140360	0.000000
H	–0.577270	5.491960	0.000000
H	–2.638160	4.311430	0.000000
O	3.035950	–1.935620	0.000000
C	1.902430	–2.406690	0.000000
N	1.774010	–3.791930	0.000000
C	0.569050	–4.409480	0.000000
C	–0.569050	–3.686150	0.000000
C	–0.422400	–2.258440	0.000000
N	0.765870	–1.662430	0.000000
N	–1.494490	–1.421890	0.000000
C	–2.860240	–1.799770	0.000000
O	–3.228820	–2.959730	0.000000
N	–3.695480	–0.748660	0.000000
H	–3.403580	0.232930	0.000000
H	–1.259320	–0.424000	0.000000
H	–1.544210	–4.140360	0.000000
H	0.577270	–5.491960	0.000000
H	2.638160	–4.311430	0.000000
H	–4.675130	–0.972370	0.000000
H	4.675130	0.972370	0.000000

Sum of electronic and thermal free energy: –1127.096052 a.u.
N_{Im}= 1 (21*i* cm^{-1})

44•44

	X	Y	Z
O	–0.619594	–3.597795	0.000000
O	–3.265348	3.205802	0.000000
C	–1.794472	–3.248941	0.000000
C	–2.090471	2.856948	0.000000
N	–2.784287	–4.241406	0.000000
N	–1.100655	3.849413	0.000000
C	–4.101468	–3.966819	0.000000
C	0.216525	3.574826	0.000000
C	–4.525997	–2.676999	0.000000
C	0.641055	2.285006	0.000000
C	–3.506380	–1.682723	0.000000
C	–0.378562	1.290730	0.000000
N	–2.207042	–1.957254	0.000000
N	–1.677901	1.565261	0.000000
N	–3.876259	–0.384872	0.000000
N	–0.008683	–0.007122	0.000000
C	–5.208842	0.003448	0.000000
C	1.323899	–0.395441	0.000000

C	–6.227154	–0.921672	0.000000
C	2.342211	0.529679	0.000000
N	–5.401798	1.332760	0.000000
N	1.516855	–1.724753	0.000000
H	–4.632554	2.006438	0.000000
H	0.747611	–2.398431	0.000000
H	–3.124810	0.323829	0.000000
H	–0.760132	–0.715822	0.000000
C	–5.973152	–2.326589	0.000000
C	2.088210	1.934596	0.000000
H	–4.807019	–4.789750	0.000000
H	0.922076	4.397757	0.000000
H	–2.445632	–5.192359	0.000000
H	–1.439311	4.800366	0.000000
O	–6.821049	–3.213186	0.000000
O	2.936107	2.821193	0.000000
H	–7.254482	–0.582572	0.000000
H	3.369539	0.190579	0.000000
H	–6.343653	1.679697	0.000000
H	2.458710	–2.071690	0.000000

Sum of electronic and thermal free energy: –1279.456152 a.u.
N_{Im}= 0

45•45

	X	Y	Z
N	1.645056	0.893785	0.000000
C	2.221343	–0.281112	0.000000
N	3.567405	–0.473592	0.000000
C	4.503502	0.551619	0.000000
C	3.884863	1.878275	0.000000
C	2.482155	1.984063	0.000000
O	5.691707	0.325927	0.000000
C	4.666557	3.029115	0.000000
N	1.890277	3.190314	0.000000
N	1.427823	–1.397266	0.000000
H	0.416719	–1.218077	0.000000
C	1.890640	–2.725218	0.000000
N	0.915840	–3.642478	0.000000
O	3.082806	–3.009059	0.000000
H	–0.416743	1.218059	0.000000
N	–1.427843	1.397267	0.000000
C	–2.221368	0.281120	0.000000
N	–1.645069	–0.893772	0.000000
C	–2.482156	–1.984056	0.000000
C	–3.884868	–1.878286	0.000000
C	–4.503520	–0.551638	0.000000
N	–3.567430	0.473586	0.000000
O	–5.691725	–0.325952	0.000000
C	–4.666544	–3.029136	0.000000
N	–1.890266	–3.190296	0.000000

H	–0.089561	–3.421129	0.000000
H	3.882301	–1.451071	0.000000
C	4.042895	4.260416	0.000000
H	5.745579	2.923767	0.000000
C	2.649660	4.276715	0.000000
H	4.602719	5.186158	0.000000
H	2.116549	5.223991	0.000000
C	–1.890637	2.725232	0.000000
O	–3.082798	3.009093	0.000000
N	–0.915828	3.642480	0.000000
H	–1.225024	4.599063	0.000000
H	0.089576	3.421129	0.000000
H	–3.882334	1.451061	0.000000
H	–5.745567	–2.923806	0.000000
C	–4.042864	–4.260431	0.000000
H	1.225046	–4.599058	0.000000
C	–2.649631	–4.276711	0.000000
H	–2.116506	–5.223979	0.000000
H	–4.602679	–5.186179	0.000000

Sum of electronic and thermal free energy: –1466.385933 a.u.
N_{Im}= 1 (12*i* cm^{-1})

46•46

	X	Y	Z
N	–2.983616	–0.558040	0.000000
N	–0.654750	2.201298	0.000000
C	–3.964022	0.326742	0.000000
C	0.325653	1.316515	0.000000
N	–5.273644	0.007477	0.000000
N	1.635277	1.635775	0.000000
C	–5.683367	–1.306967	0.000000
C	2.045003	2.950218	0.000000
C	–4.701802	–2.295600	0.000000
C	1.063440	3.938853	0.000000
C	–3.283991	–1.895945	0.000000
C	–0.354372	3.539202	0.000000
N	–6.993118	–1.539151	0.000000
N	3.354754	3.182401	0.000000
O	–2.400250	–2.750097	0.000000
O	–1.238109	4.393356	0.000000
N	–3.625461	1.646706	0.000000
N	–0.012911	–0.003446	0.000000
H	–2.612687	1.835504	0.000000
H	–1.025685	–0.192246	0.000000
C	–4.538026	2.719257	0.000000
C	0.899660	–1.075988	0.000000
N	–3.960336	3.924125	0.000000
N	0.321978	–2.280861	0.000000
O	–5.751664	2.542227	0.000000
O	2.113295	–0.898939	0.000000

H	–2.944519	4.076042	0.000000
H	–0.693838	–2.432785	0.000000
H	–5.942553	0.785989	0.000000
H	2.304186	0.857264	0.000000
H	–4.585376	4.711357	0.000000
H	0.947025	–3.068087	0.000000
C	–5.120463	–3.623972	0.000000
C	1.482102	5.267225	0.000000
H	–4.373010	–4.408431	0.000000
H	0.734650	6.051685	0.000000
C	–6.476207	–3.890345	0.000000
C	2.837846	5.533596	0.000000
H	–6.853446	–4.904825	0.000000
H	3.215086	6.548075	0.000000
C	–7.365380	–2.812568	0.000000
C	3.727018	4.455818	0.000000
H	–8.436997	–2.988837	0.000000
H	4.798635	4.632086	0.000000

Sum of electronic and thermal free energy: –1466.390904 a.u.
N_{Im}= 0

45•46

	X	Y	Z
N	1.703897	–0.556572	0.000000
C	0.613643	–1.298009	0.000000
N	0.610061	–2.645804	0.000000
C	1.788539	–3.358201	0.000000
C	2.982349	–2.641208	0.000000
C	2.932843	–1.169040	0.000000
N	1.700235	–4.685310	0.000000
O	3.972774	–0.516182	0.000000
N	–0.591311	–0.655277	0.000000
H	–0.539825	0.372204	0.000000
C	–1.845882	–1.290955	0.000000
N	–2.883553	–0.446540	0.000000
O	–1.962780	–2.511108	0.000000
H	–2.790267	0.579576	0.000000
H	–0.304055	–3.111542	0.000000
C	4.172478	–3.365047	0.000000
H	5.112873	–2.826809	0.000000
C	4.106845	–4.745084	0.000000
H	5.001736	–5.353854	0.000000
C	2.847787	–5.351153	0.000000
H	2.763044	–6.433818	0.000000
H	1.794070	1.457472	0.000000
N	1.856881	2.483896	0.000000
C	0.657536	3.138930	0.000000
N	–0.442997	2.426892	0.000000
C	–1.624068	3.127396	0.000000
C	–1.685798	4.533042	0.000000

C	–0.441549	5.305221	0.000000
N	0.687673	4.498536	0.000000
O	–0.360534	6.512101	0.000000
C	–2.921009	5.172416	0.000000
N	–2.752351	2.396047	0.000000
C	3.124184	3.097975	0.000000
O	3.263095	4.316306	0.000000
N	4.146948	2.237224	0.000000
H	4.046518	1.215883	0.000000
H	1.622667	4.925089	0.000000
H	–2.944273	6.256346	0.000000
C	–4.070031	4.407224	0.000000
C	–3.920969	3.022126	0.000000
H	–4.798706	2.380787	0.000000
H	–5.055623	4.853353	0.000000
H	5.064110	2.648614	0.000000
H	–3.792245	–0.876534	0.000000

Sum of electronic and thermal free energy: –1466.386608 a.u.
N_{Im}= 1 (7*i* cm^{-1})

ADDA-DAAD arrays

4•5

	X	Y	Z
N	0.010343	–0.004250	0.000000
C	–1.135043	–0.652724	0.000000
C	–1.241091	–2.076613	0.000000
C	–0.088731	–2.801074	0.000000
C	1.158983	–2.138761	0.000000
C	1.158944	–0.717699	0.000000
N	2.307505	–0.004186	0.000000
C	3.452926	–0.652596	0.000000
C	3.559054	–2.076479	0.000000
C	2.406735	–2.801004	0.000000
H	–2.213788	–2.554258	0.000000
H	–0.117767	–3.886593	0.000000
H	2.435831	–3.886522	0.000000
H	4.531778	–2.554070	0.000000
N	4.587388	0.105010	0.000000
H	4.490167	1.104837	0.000000
N	–2.269546	0.104819	0.000000
H	–2.172382	1.104651	0.000000
H	–3.182632	–0.307775	0.000000
H	5.500496	–0.307532	0.000000

Sum of electronic and thermal free energy: –1261.747115 a.u.
N_{Im}= 1 (33*i* cm^{-1})

4•6

	X	Y	Z
C	–0.010473	0.697026	0.000000

N	–1.192606	–0.016374	0.000000
N	1.132077	–0.078187	0.000000
C	–2.463723	0.566698	0.000000
C	2.432383	0.436512	0.000000
C	–2.716412	1.949361	0.000000
C	2.758190	1.803794	0.000000
C	–4.031138	2.375920	0.000000
C	4.093725	2.159885	0.000000
N	–3.463429	–0.315527	0.000000
N	3.383795	–0.497591	0.000000
H	–4.239687	3.440104	0.000000
H	4.358530	3.211483	0.000000
C	–5.072250	1.453989	0.000000
C	5.084375	1.183932	0.000000
C	–4.722950	0.117890	0.000000
C	4.664568	–0.131717	0.000000
H	–5.485754	–0.656797	0.000000
H	5.385127	–0.945846	0.000000
H	–6.110815	1.758190	0.000000
H	6.137638	1.432513	0.000000
H	–1.899464	2.649327	0.000000
H	1.979592	2.546183	0.000000
H	–1.179361	–1.042643	0.000000
H	1.064313	–1.102303	0.000000
O	0.021890	1.914115	0.000000
N	1.035399	–3.337110	0.000000
C	2.169416	–4.031957	0.000000
C	2.219180	–5.460372	0.000000
C	1.048311	–6.145456	0.000000
C	–0.173676	–5.440901	0.000000
C	–0.135900	–4.020185	0.000000
N	–1.269245	–3.275831	0.000000
C	–2.438585	–3.909432	0.000000
C	–2.564186	–5.333185	0.000000
C	–1.431378	–6.079522	0.000000
N	–3.560822	–3.161090	0.000000
H	3.177882	–5.965092	0.000000
H	1.037591	–7.231284	0.000000
N	3.329836	–3.344309	0.000000
H	–1.478375	–7.164385	0.000000
H	–3.548355	–5.786245	0.000000
H	–3.484344	–2.140018	0.000000
H	3.307727	–2.320615	0.000000
H	4.202140	–3.838562	0.000000
H	–4.458159	–3.608289	0.000000

Sum of electronic and thermal free energy: –1247.788395 a.u.
N_{Im}= 4 (70*i* cm^{-1}, 60*i* cm^{-1}, 28*i* cm^{-1}, 22*i* cm^{-1})

47•48

	X	Y	Z

O	–3.378955	1.982498	0.000000
C	–2.214018	4.043141	0.000000
C	–0.980318	4.601276	0.000000
H	–0.860688	5.679740	0.000000
N	0.182989	3.896509	0.000000
C	0.087688	2.590540	0.000000
N	–1.104836	1.938537	0.000000
C	–2.327360	2.613427	0.000000
N	1.201192	1.796823	0.000000
C	2.550306	2.192657	0.000000
O	3.416069	1.321421	0.000000
N	2.832725	3.497321	0.000000
C	4.209845	3.947758	0.000000
H	4.211774	5.037132	0.000000
H	1.070408	0.776350	0.000000
H	–1.143897	0.902197	0.000000
H	2.047418	4.141875	0.000000
N	–1.416396	–1.077552	0.000000
C	–2.622415	–1.630092	0.000000
C	–2.850693	–3.032390	0.000000
C	–1.765200	–3.851245	0.000000
C	–0.466479	–3.303968	0.000000
C	–0.330847	–1.895299	0.000000
N	0.888851	–1.297220	0.000000
C	1.966667	–2.069904	0.000000
C	1.925269	–3.490317	0.000000
C	0.704324	–4.088557	0.000000
N	3.176682	–1.399099	0.000000
C	4.448509	–1.911308	0.000000
O	4.773261	–3.075795	0.000000
N	–3.682944	–0.741559	0.000000
C	–5.029437	–1.004025	0.000000
O	–5.567707	–2.086249	0.000000
H	3.134993	–0.372767	0.000000
H	–3.449063	0.259053	0.000000
H	–3.863471	–3.403697	0.000000
H	–1.888597	–4.929329	0.000000
H	0.620594	–5.170422	0.000000
H	2.849490	–4.046727	0.000000
H	–3.121502	4.628749	0.000000
H	5.186493	–1.092755	0.000000
H	–5.599439	–0.060877	0.000000
H	4.739712	3.589356	0.885194
H	4.739712	3.589356	–0.885194

Sum of electronic and thermal free energy: –1358.026810 a.u.
N_{Im}= 1 (6*i* cm^{-1})

47•49

	X	Y	Z
O	–4.397741	–2.549613	0.000000

C	–5.384202	–1.815054	0.000000
C	–6.750029	–2.279425	0.000000
C	–7.780434	–1.400888	0.000000
C	–7.560801	0.005398	0.000000
C	–6.243835	0.446490	0.000000
N	–5.213969	–0.434901	0.000000
N	–5.952582	1.770364	0.000000
C	–6.919738	2.769569	0.000000
H	–4.961267	2.075313	0.000000
H	–4.238968	–0.081243	0.000000
H	–6.896044	–3.350539	0.000000
H	–8.803835	–1.762812	0.000000
N	–3.116604	2.715121	0.000000
C	–2.854836	4.015479	0.000000
C	–1.539683	4.553949	0.000000
C	–0.496262	3.681390	0.000000
C	–0.734116	2.291859	0.000000
C	–2.074844	1.842813	0.000000
N	–2.381068	0.519023	0.000000
C	–1.388908	–0.361357	0.000000
C	–0.014736	0.000901	0.000000
C	0.292663	1.325888	0.000000
N	–1.773223	–1.690837	0.000000
H	–1.405678	5.624254	0.000000
H	0.525563	4.046491	0.000000
N	–3.962358	4.845307	0.000000
H	1.328257	1.649877	0.000000
H	0.736873	–0.772785	0.000000
O	–6.574673	3.950080	0.000000
C	–8.289729	2.317635	0.000000
H	–9.051418	3.084732	0.000000
C	–8.583131	0.995714	0.000000
H	–9.618068	0.668234	0.000000
C	–4.010553	6.217338	0.000000
H	–4.887553	4.396214	0.000000
C	–0.985344	–2.815132	0.000000
H	–2.782273	–1.889574	0.000000
H	–5.057905	6.559608	0.000000
O	–3.077077	6.984598	0.000000
H	–1.615283	–3.719162	0.000000
O	0.221943	–2.865405	0.000000

Sum of electronic and thermal free energy: –1323.526414 a.u.
N_{Im}= 0

4•48

	X	Y	Z
O	2.462300	–2.923918	0.000000
C	2.786295	–1.742065	0.000000
C	4.138492	–1.259252	0.000000
C	4.355848	0.076426	0.000000

N	3.372546	1.013997	0.000000
C	2.132887	0.583146	0.000000
N	1.813603	–0.738243	0.000000
N	1.082669	1.459625	0.000000
C	1.131912	2.865562	0.000000
O	0.079982	3.496948	0.000000
N	2.329693	3.462250	0.000000
C	2.424169	4.906336	0.000000
H	3.479217	5.179226	0.000000
H	3.147122	2.858348	0.000000
H	0.121787	1.077050	0.000000
H	0.817528	–1.050292	0.000000
H	4.939621	–1.983723	0.000000
H	5.365943	0.473826	0.000000
N	–1.766534	0.390094	0.000000
C	–2.788310	1.247157	0.000000
C	–4.155840	0.828671	0.000000
C	–4.427155	–0.499940	0.000000
C	–3.367760	–1.432193	0.000000
C	–2.037909	–0.939507	0.000000
N	–0.967637	–1.775569	0.000000
C	–1.184500	–3.091656	0.000000
C	–2.495324	–3.662695	0.000000
C	–3.565277	–2.829397	0.000000
N	–0.122907	–3.918495	0.000000
H	–0.269101	–4.910833	0.000000
H	–4.943016	1.572824	0.000000
H	–5.451987	–0.858499	0.000000
N	–2.520029	2.565621	0.000000
H	–3.275922	3.224862	0.000000
H	–4.576891	–3.223776	0.000000
H	–2.609391	–4.739871	0.000000
H	0.833249	–3.557773	0.000000
H	–1.558426	2.910225	0.000000
H	1.945182	5.332475	–0.884663
H	1.945182	5.332475	0.884663

Sum of electronic and thermal free energy: –1131.384523 a.u.
N_{Im}= 1 (32*i* cm^{-1})

4•49

	X	Y	Z
O	3.598830	–0.649536	0.000000
C	3.722727	0.573228	0.000000
C	4.994741	1.256937	0.000000
C	5.054638	2.608933	0.000000
C	3.876222	3.405377	0.000000
C	2.652082	2.744030	0.000000
N	2.594822	1.388731	0.000000
N	1.487136	3.439052	0.000000
C	1.423446	4.829428	0.000000

H	0.579264	2.924821	0.000000
H	1.667032	0.911416	0.000000
H	5.877390	0.632617	0.000000
H	6.016649	3.112354	0.000000
N	–1.092375	2.033118	0.000000
C	–2.220965	2.743390	0.000000
C	–3.515750	2.136340	0.000000
C	–3.597804	0.782112	0.000000
C	–2.419310	0.004892	0.000000
C	–1.172801	0.678237	0.000000
N	0.004399	0.002639	0.000000
C	–0.020337	–1.330661	0.000000
C	–1.237898	–2.080639	0.000000
C	–2.415459	–1.406781	0.000000
N	1.150345	–1.994489	0.000000
H	1.149181	–2.997681	0.000000
H	–4.400030	2.761907	0.000000
H	–4.563003	0.284942	0.000000
N	–2.134307	4.086388	0.000000
H	–2.973946	4.635389	0.000000
H	–3.360434	–1.941377	0.000000
H	–1.199560	–3.163136	0.000000
H	2.047703	–1.503443	0.000000
H	–1.231654	4.567640	0.000000
O	0.332910	5.396210	0.000000
C	2.692531	5.518522	0.000000
H	2.654163	6.598965	0.000000
C	3.856153	4.827528	0.000000
H	4.804560	5.356120	0.000000

Sum of electronic and thermal free energy: –1096.881019 a.u.
N_{Im}= 1 (22*i* cm^{-1})

ADAA-DADD arrays

50•51

	X	Y	Z
N	–3.281992	1.666702	0.000000
C	–3.212903	0.308256	0.000000
C	–4.398032	–0.446386	0.000000
C	–4.287372	–1.818418	0.000000
C	–3.041082	–2.427763	0.000000
C	–1.920413	–1.596637	0.000000
N	–1.993401	–0.252759	0.000000
N	–0.618193	–2.092893	0.000000
C	–0.236061	–3.432656	0.000000
O	–1.018064	–4.367689	0.000000
N	1.108715	–3.619222	0.000000
H	1.411114	–4.576420	0.000000
H	1.804723	–2.882023	0.000000
H	0.108011	–1.385429	0.000000

H	–2.920600	–3.497315	0.000000
H	–5.180205	–2.434781	0.000000
H	–5.360584	0.050800	0.000000
H	–4.177457	2.116584	0.000000
H	–2.450006	2.238015	0.000000
O	3.259283	–1.749133	0.000000
C	3.142786	–0.538602	0.000000
N	4.309852	0.237152	0.000000
C	4.284063	1.582072	0.000000
C	3.103990	2.244090	0.000000
C	1.915013	1.443023	0.000000
N	1.950754	0.128078	0.000000
N	0.640987	1.970606	0.000000
C	0.155040	3.274102	0.000000
O	–1.044685	3.439692	0.000000
H	3.108052	3.315757	0.000000
H	5.239362	2.091505	0.000000
H	5.177093	–0.278838	0.000000
H	–0.101992	1.258868	0.000000
C	1.066517	4.474695	0.000000
H	0.422463	5.350865	0.000000
H	1.696827	4.498126	0.890953
H	1.696827	4.498126	–0.890953

Sum of electronic and thermal free energy: –1075.049726 a.u.
N_{Im}= 1 (153*i* cm^{-1})

52•53

	X	Y	Z
O	3.379677	1.593029	0.000000
N	–3.294409	–1.766832	0.000000
C	3.119239	0.405329	0.000000
C	–3.121084	–0.423180	0.000000
N	4.191167	–0.512333	0.000000
C	–4.255047	0.423954	0.000000
C	4.023604	–1.843201	0.000000
C	–4.062153	1.777741	0.000000
C	2.766798	–2.370815	0.000000
C	–2.766630	2.303515	0.000000
C	1.687051	–1.420456	0.000000
C	–1.713402	1.390588	0.000000
N	1.862572	–0.116653	0.000000
N	–1.866572	0.050010	0.000000
N	0.415507	–1.894762	0.000000
N	–0.423189	1.861732	0.000000
C	0.085310	–3.248263	0.000000
C	–0.143160	3.206290	0.000000
C	1.199621	–4.199599	0.000000
C	–1.146297	4.141091	0.000000
O	–1.077466	–3.603674	0.000000
N	1.175462	3.528074	0.000000

H	1.917009	2.837377	0.000000
H	–0.370323	–1.204821	0.000000
H	0.340285	1.186955	0.000000
C	2.471516	–3.779202	0.000000
C	–2.528844	3.764094	0.000000
H	4.916994	–2.456746	0.000000
H	–4.890089	2.478262	0.000000
H	5.112062	–0.097925	0.000000
H	–5.247601	–0.010253	0.000000
O	–3.468226	4.559929	0.000000
H	0.924838	–5.245414	0.000000
H	–0.897802	5.194642	0.000000
H	1.428551	4.498141	0.000000
H	3.294644	–4.486369	0.000000
H	–2.512392	–2.410674	0.000000
H	–4.224199	–2.142193	0.000000

Sum of electronic and thermal free energy: –1188.153527 a.u.
N_{Im}= 2 (83*i* cm^{-1}, 50*i* cm^{-1})

50•54

	X	Y	Z
N	1.011814	4.886324	0.000000
C	2.287891	4.420833	0.000000
C	3.352151	5.338728	0.000000
C	4.634243	4.842267	0.000000
C	4.862112	3.473487	0.000000
C	3.748766	2.635287	0.000000
N	2.478210	3.089050	0.000000
N	3.861314	1.246212	0.000000
C	5.042232	0.508147	0.000000
O	6.159142	0.994034	0.000000
N	4.845600	–0.837196	0.000000
H	5.685034	–1.388109	0.000000
H	3.943257	–1.303983	0.000000
H	2.986883	0.731841	0.000000
H	5.853127	3.054238	0.000000
H	5.479695	5.521901	0.000000
H	3.149977	6.402873	0.000000
H	0.853886	5.876244	0.000000
H	0.207601	4.274086	0.000000
N	2.424773	–2.514794	0.000000
C	1.188557	–1.965704	0.000000
C	0.025645	–2.780048	0.000000
C	–1.223923	–2.133781	0.000000
C	–1.267504	–0.770598	0.000000
C	–0.040705	–0.040612	0.000000
N	1.140075	–0.610656	0.000000
N	–0.092980	1.336892	0.000000
C	–1.265771	2.050401	0.000000
C	–2.564016	–0.067148	0.000000

H	–2.153108	–2.694284	0.000000
C	0.179593	–4.183538	0.000000
H	0.792006	1.880356	0.000000
O	–1.317882	3.260586	0.000000
N	–2.437006	1.307358	0.000000
O	–3.641432	–0.613417	0.000000
H	–3.288225	1.852902	0.000000
H	–0.701664	–4.816246	0.000000
C	1.439330	–4.712825	0.000000
H	1.611032	–5.781252	0.000000
C	2.533086	–3.821957	0.000000
H	3.546225	–4.215797	0.000000

Sum of electronic and thermal free energy: –1281.624355 a.u.
N_{Im}= 2 (93*i* cm^{-1}, 39*i* cm^{-1})

ADAD-DADA arrays

55•55

	X	Y	Z
N	–1.999703	–0.054716	0.000000
C	–2.026860	1.280153	0.000000
N	–3.101045	2.053052	0.000000
C	–4.272424	1.412864	0.000000
C	–4.393182	0.043172	0.000000
C	–3.188639	–0.673364	0.000000
H	–5.156935	2.042740	0.000000
H	–5.345272	–0.461995	0.000000
N	–3.126635	–2.047858	0.000000
H	–2.187478	–2.464972	0.000000
C	–4.171077	–2.940320	0.000000
O	–5.348664	–2.674747	0.000000
N	–0.769334	1.880755	0.000000
H	0.023822	1.238798	0.000000
C	–0.411899	3.210402	0.000000
O	0.781000	3.485780	0.000000
H	–0.023822	–1.238798	0.000000
N	0.769334	–1.880755	0.000000
C	2.026860	–1.280153	0.000000
N	1.999703	0.054716	0.000000
C	3.188639	0.673364	0.000000
C	4.393182	–0.043172	0.000000
C	4.272424	–1.412864	0.000000
N	3.101045	–2.053052	0.000000
H	5.156935	–2.042740	0.000000
H	5.345272	0.461995	0.000000
C	0.411899	–3.210402	0.000000
O	–0.781000	–3.485780	0.000000
N	3.126635	2.047858	0.000000
H	2.187478	2.464972	0.000000
C	4.171077	2.940320	0.000000

O	5.348664	2.674747	0.000000
H	–3.793496	–3.975308	0.000000
H	3.793496	3.975308	0.000000
C	1.437904	–4.304238	0.000000
C	–1.437904	4.304238	0.000000
H	–0.898050	5.249157	0.000000
H	–2.087283	4.226965	–0.871924
H	–2.087283	4.226965	0.871924
H	0.898050	–5.249157	0.000000
H	2.087283	–4.226965	–0.871924
H	2.087283	–4.226965	0.871924

Sum of electronic and thermal free energy: –1281.821812 a.u.
N_{Im}= 1 (17 cm^{-1})

56•56

	X	Y	Z
N	0.076967	2.001447	0.000000
C	1.407611	1.884125	0.000000
N	2.285907	2.884159	0.000000
C	1.767568	4.116311	0.000000
C	0.420793	4.373870	0.000000
C	–0.420211	3.247258	0.000000
H	2.484204	4.931733	0.000000
H	0.015958	5.371739	0.000000
N	–1.789824	3.324049	0.000000
H	–2.289853	2.424459	0.000000
C	–2.577047	4.466256	0.000000
O	–2.133779	5.593863	0.000000
C	–4.055961	4.165911	0.000000
H	–4.323556	3.571842	0.876333
H	–4.323556	3.571842	–0.876333
H	–4.601398	5.107025	0.000000
N	1.886125	0.587038	0.000000
H	1.194189	–0.161271	0.000000
C	3.199640	0.120706	0.000000
O	3.398884	–1.095898	0.000000
N	4.199411	1.009287	0.000000
H	3.940486	1.991849	0.000000
C	5.576815	0.565328	0.000000
H	5.797531	–0.036017	0.885089
H	5.797531	–0.036017	–0.885089
H	6.219115	1.445530	0.000000
H	–1.194186	0.161288	0.000000
N	–1.886122	–0.587022	0.000000
C	–1.407613	–1.884107	0.000000
N	–0.076968	–2.001433	0.000000
C	0.420206	–3.247241	0.000000
C	–0.420797	–4.373853	0.000000
C	–1.767573	–4.116291	0.000000
N	–2.285912	–2.884136	0.000000

H	–2.484213	–4.931712	0.000000
H	–0.015957	–5.371720	0.000000
C	–3.199638	–0.120697	0.000000
O	–3.398888	1.095905	0.000000
N	–4.199400	–1.009289	0.000000
H	–3.940462	–1.991849	0.000000
C	–5.576810	–0.565348	0.000000
H	–5.797533	0.035994	0.885089
H	–5.797533	0.035994	–0.885089
H	–6.219099	–1.445558	0.000000
N	1.789818	–3.324036	0.000000
H	2.289842	–2.424445	0.000000
C	2.577034	–4.466244	0.000000
O	2.133756	–5.593848	0.000000
C	4.055950	–4.165912	0.000000
H	4.323550	–3.571844	0.876334
H	4.323550	–3.571844	–0.876334
H	4.601379	–5.107032	0.000000

Sum of electronic and thermal free energy: –1471.134235 a.u.
N_{Im}= 2 (102*i* cm^{-1}, 102*i* cm^{-1})

57•57

	X	Y	Z
N	0.602967	1.779116	0.000000
C	0.503240	3.107850	0.000000
C	1.643252	3.933329	0.000000
C	2.866353	3.312238	0.000000
N	2.976104	1.967074	0.000000
C	1.846416	1.274638	0.000000
N	1.898414	–0.103737	0.000000
C	2.989767	–0.960917	0.000000
O	2.792159	–2.181315	0.000000
N	4.219885	–0.437009	0.000000
C	5.387753	–1.292368	0.000000
H	6.274673	–0.659171	0.000000
H	5.406587	–1.932928	0.884638
H	5.406587	–1.932928	–0.884638
H	4.282620	0.577407	0.000000
H	1.001215	–0.598156	0.000000
C	4.155805	4.074876	0.000000
H	1.531506	5.008088	0.000000
O	–0.673374	3.678410	0.000000
H	–1.428600	3.024795	0.000000
O	–2.793527	2.181859	0.000000
C	–2.991124	0.961459	0.000000
N	–1.899764	0.104294	0.000000
N	–4.221234	0.437529	0.000000
C	–1.847765	–1.274079	0.000000
N	–2.977465	–1.966501	0.000000
C	–2.867725	–3.311663	0.000000

C	–1.644628	–3.932765	0.000000
C	–0.504609	–3.107298	0.000000
N	–0.604324	–1.778564	0.000000
O	0.672002	–3.677867	0.000000
C	–5.389117	1.292867	0.000000
H	–6.276028	0.659658	0.000000
H	–5.407962	1.933427	0.884638
H	–5.407962	1.933427	–0.884638
H	–4.283947	–0.576889	0.000000
H	–1.002568	0.598718	0.000000
C	–4.157183	–4.074292	0.000000
H	–1.532891	–5.007525	0.000000
H	1.427237	–3.024260	0.000000
H	–3.987064	–5.151189	0.000000
H	–4.745282	–3.807322	–0.881656
H	–4.745282	–3.807322	0.881656
H	3.985678	5.151772	0.000000
H	4.743906	3.807914	–0.881657
H	4.743906	3.807914	0.881657

Sum of electronic and thermal free energy: –1284.254194 a.u.
N_{Im}= 0

58•58

	X	Y	Z
N	–2.578958	0.644514	0.000000
C	–2.158457	–0.620220	0.000000
N	–0.874981	–1.005699	0.000000
C	0.000194	0.000339	0.000000
N	–0.273624	1.281750	0.000000
C	–1.599920	1.570090	0.000000
H	1.050851	–0.278622	0.000000
N	–1.937209	2.854572	0.000000
H	–2.917822	3.151009	0.000000
N	–3.141347	–1.574034	0.000000
H	–4.105952	–1.229192	0.000000
C	–3.042314	–2.971512	0.000000
O	–4.074873	–3.638349	0.000000
N	–1.823625	–3.524352	0.000000
H	–1.028152	–2.893126	0.000000
C	–1.671940	–4.963917	0.000000
H	–2.133474	–5.408386	0.884825
H	–2.133474	–5.408386	–0.884825
H	–0.607048	–5.195001	0.000000
H	–4.571491	1.229195	0.000000
N	–5.536094	1.574039	0.000000
C	–6.518984	0.620223	0.000000
N	–6.098485	–0.644510	0.000000
C	–7.077528	–1.570085	0.000000
N	–8.403820	–1.281742	0.000000
C	–8.677636	–0.000330	0.000000

N	–7.802461	1.005706	0.000000
H	–9.728292	0.278632	0.000000
C	–5.635127	2.971518	0.000000
O	–4.602571	3.638357	0.000000
N	–6.853821	3.524353	0.000000
H	–7.649291	2.893124	0.000000
C	–7.005512	4.963918	0.000000
H	–6.543982	5.408391	0.884826
H	–6.543982	5.408391	–0.884826
H	–8.070405	5.194994	0.000000
N	–6.740233	–2.854565	0.000000
H	–5.759619	–3.150998	0.000000
H	–1.191552	3.528348	0.000000
H	–7.485888	–3.528345	0.000000

Sum of electronic and thermal free energy: –1198.024420 a.u.
N_{Im}= 0

59•59

	X	Y	Z
N	–0.049490	–1.453340	0.000000
C	1.164390	–2.001950	0.000000
N	2.319990	–1.340800	0.000000
C	2.184030	–0.015280	0.000000
N	1.060470	0.663690	0.000000
C	–0.054530	–0.104210	0.000000
H	3.105410	0.561710	0.000000
N	–1.223440	0.529480	0.000000
H	–2.106510	0.017590	0.000000
N	1.179090	–3.384470	0.000000
H	0.257270	–3.832660	0.000000
C	2.240890	–4.271100	0.000000
O	1.989720	–5.465760	0.000000
C	3.664090	–3.795650	0.000000
H	–1.902340	–2.528120	0.000000
N	–2.824160	–2.976310	0.000000
C	–2.809460	–4.358830	0.000000
N	–1.595580	–4.907430	0.000000
C	–1.590530	–6.256570	0.000000
N	–2.705540	–7.024470	0.000000
C	–3.829100	–6.345500	0.000000
N	–3.965050	–5.019980	0.000000
H	–4.750470	–6.922490	0.000000
C	–3.885960	–2.089680	0.000000
O	–3.634790	–0.895010	0.000000
C	–5.309160	–2.565130	0.000000
N	–0.421630	–6.890250	0.000000
H	0.461440	–6.378370	0.000000
H	–1.206340	1.534270	0.000000
H	–0.438730	–7.895040	0.000000
H	4.296070	–4.681680	0.000000

H	3.865900	–3.173930	–0.872040
H	3.865900	–3.173930	0.872040
H	–5.941140	–1.679100	0.000000
H	–5.510970	–3.186850	–0.872040
H	–5.510970	–3.186850	0.872040

Sum of electronic and thermal free energy: –1087.310177 a.u.
N_{Im}= 0

3. Monomers

1

	X	Y	Z
C	0.222270	–1.412240	0.000000
C	–1.041358	–2.095210	0.000000
C	–2.203006	–1.341481	0.000000
N	–2.351771	0.005192	0.000000
C	–1.208834	0.634271	0.000000
N	0.002778	–0.000040	0.000000
O	1.354987	–1.832580	0.000000
N	–1.196389	1.992315	0.000000
N	–1.328733	–3.442417	0.000000
C	–2.626129	–3.500169	0.000000
N	–3.215817	–2.253580	0.000000
H	–2.081995	2.465255	0.000000
H	–0.349889	2.529068	0.000000
H	–3.215514	–4.404958	0.000000
H	0.857792	0.537611	0.000000
H	–4.198743	–2.038138	0.000000

Sum of electronic and thermal free energy: –542.443569 a.u.
N_{Im}= 1 (327*i* cm^{-1})

2

	X	Y	Z
C	0.020881	1.309741	0.000000
N	–0.019586	–0.001213	0.000000
C	1.138366	–0.727788	0.000000
O	1.208099	–1.936817	0.000000
N	2.345723	0.016302	0.000000
C	2.386205	1.366750	0.000000
C	1.237877	2.077771	0.000000
N	–1.164091	1.963033	0.000000
H	3.366682	1.827174	0.000000
H	1.240297	3.158064	0.000000
H	–2.006994	1.414302	0.000000
H	–1.220004	2.964194	0.000000
H	3.189856	–0.534492	0.000000

Sum of electronic and thermal free energy: –394.846744 a.u.
N_{Im}= 1 (56*i* cm^{-1})

3

	X	Y	Z
O	2.515699	–2.491543	0.000000
C	2.763977	–1.303122	0.000000
C	4.136961	–0.783455	0.000000
C	4.379014	0.539362	0.000000
N	3.303465	1.406011	0.000000
C	2.045956	0.899536	0.000000
N	1.735118	–0.349514	0.000000
N	0.989172	1.806453	0.000000
C	1.063966	3.190186	0.000000
O	2.125446	3.799353	0.000000
N	–0.134782	3.820880	0.000000
H	–0.987639	3.289800	0.000000
H	0.097405	1.334386	0.000000
H	3.400772	2.419104	0.000000
C	5.728920	1.181363	0.000000
H	4.948233	–1.498620	0.000000
C	–0.205291	5.270389	0.000000
H	6.509460	0.421859	0.000000
H	5.855832	1.812597	–0.884274
H	5.855832	1.812597	0.884274
H	–1.254658	5.563026	0.000000
H	0.280046	5.684261	0.886014
H	0.280046	5.684261	–0.886014

Sum of electronic and thermal free energy: –642.099321 a.u.
N_{Im}= 1 (67*i* cm^{-1})

4

	X	Y	Z
N	0.010343	–0.004250	0.000000
C	–1.135043	–0.652724	0.000000
C	–1.241091	–2.076613	0.000000
C	–0.088731	–2.801074	0.000000
C	1.158983	–2.138761	0.000000
C	1.158944	–0.717699	0.000000
N	2.307505	–0.004186	0.000000
C	3.452926	–0.652596	0.000000
C	3.559054	–2.076479	0.000000
C	2.406735	–2.801004	0.000000
H	–2.213788	–2.554258	0.000000
H	–0.117767	–3.886593	0.000000
H	2.435831	–3.886522	0.000000
H	4.531778	–2.554070	0.000000
N	4.587388	0.105010	0.000000
H	4.490167	1.104837	0.000000
N	–2.269546	0.104819	0.000000
H	–2.172382	1.104651	0.000000
H	–3.182632	–0.307775	0.000000
H	5.500496	–0.307532	0.000000

Sum of electronic and thermal free energy: –528.537149 a.u.

N_{Im}= 2 (296*i* cm^{-1}, 293*i* cm^{-1})

5

	X	Y	Z
C	–0.507982	1.353615	0.000000
N	0.478515	2.303738	0.000000
C	0.392325	3.722922	0.000000
O	1.431074	4.347219	0.000000
N	–0.845894	4.241780	0.000000
H	1.442474	2.007926	0.000000
N	–0.058608	0.054472	0.000000
C	–0.902809	–1.058642	0.000000
H	0.929391	–0.157736	0.000000
O	–0.445351	–2.178659	0.000000
C	–2.319702	–0.694596	0.000000
N	–1.757553	1.675836	0.000000
C	–3.311867	–1.674178	0.000000
C	–2.690954	0.662025	0.000000
N	–3.973883	1.047288	0.000000
C	–4.630269	–1.272822	0.000000
H	–3.021271	–2.718444	0.000000
H	–5.442472	–1.988202	0.000000
C	–4.898315	0.100451	0.000000
H	–5.927669	0.449256	0.000000
H	–0.918179	5.243818	0.000000
H	–1.657943	3.632814	0.000000

Sum of electronic and thermal free energy: –733.175636 a.u.
N_{Im}= 0

6

	X	Y	Z
C	–0.922016	1.544310	0.000000
N	0.136538	2.429111	0.000000
C	0.099142	3.827580	0.000000
C	–1.076175	4.583918	0.000000
H	1.083491	2.080236	0.000000
N	–0.498756	0.231199	0.000000
C	–1.276490	–0.931661	0.000000
H	0.488298	0.021061	0.000000
N	–0.533139	–2.036810	0.000000
C	–2.674080	–0.944313	0.000000
O	–2.087798	1.881272	0.000000
C	–1.157822	–3.212011	0.000000
H	–0.514914	–4.087174	0.000000
C	–2.537540	–3.344661	0.000000
H	–2.997312	–4.324645	0.000000
C	–3.297748	–2.180582	0.000000
H	–4.380878	–2.230932	0.000000
H	–3.227626	–0.018290	0.000000
C	–0.944096	5.962279	0.000000

H	–2.038406	4.096024	0.000000
N	1.317476	4.365714	0.000000
C	1.416115	5.692966	0.000000
H	2.426794	6.090167	0.000000
C	0.319935	6.541262	0.000000
H	0.453902	7.615418	0.000000
H	–1.833334	6.582732	0.000000

Sum of electronic and thermal free energy: –719.239309 a.u.
N_{Im}= 0

7

	X	Y	Z
C	–1.094624	–2.190673	0.000000
C	–1.149503	–0.757308	0.000000
N	–2.294356	–0.079474	0.000000
C	–3.439208	–0.757308	0.000000
C	–3.494088	–2.190673	0.000000
C	–2.294356	–2.891175	0.000000
N	–0.002867	–0.003494	0.000000
N	–4.585845	–0.003494	0.000000
C	–4.771888	–2.821298	0.000000
H	–2.294356	–3.977821	0.000000
C	0.183176	–2.821298	0.000000
C	1.137045	–0.626899	0.000000
C	1.296302	–2.046209	0.000000
C	–5.725757	–0.626898	0.000000
C	–5.885014	–2.046209	0.000000
H	–4.831266	–3.905036	0.000000
H	–6.879783	–2.474374	0.000000
H	0.242554	–3.905036	0.000000
H	2.291071	–2.474375	0.000000
H	–6.615370	–0.000033	0.000000
H	2.026659	–0.000033	0.000000

Sum of electronic and thermal free energy: –587.439877 a.u.
N_{Im}= 0

8

	X	Y	Z
N	1.261290	2.044855	0.000000
C	0.044140	1.386196	0.000000
C	2.478895	1.387037	0.000000
N	–1.039472	2.192514	0.000000
C	0.000990	0.016682	0.000000
C	1.262279	–0.818204	0.000000
C	2.522991	0.017553	0.000000
N	3.561949	2.194104	0.000000
C	–1.284348	–0.627339	0.000000
C	3.808773	–0.625581	0.000000
O	–1.202105	–1.976393	0.000000
O	–2.386648	–0.085714	0.000000

H	–2.109568	–2.299573	0.000000
O	3.727461	–1.974691	0.000000
O	4.910700	–0.083196	0.000000
H	4.635147	–2.297245	0.000000
H	1.260943	3.050143	0.000000
H	4.466959	1.734722	0.000000
H	3.482635	3.193584	0.000000
H	–1.944163	1.732506	0.000000
H	–0.960848	3.192049	0.000000
H	1.262509	–1.483964	0.869638
H	1.262509	–1.483964	–0.869638

Sum of electronic and thermal free energy: –737.211225 a.u.
N_{Im}= 3 (393*i* cm^{-1}, 325*i* cm^{-1}, 36*i* cm^{-1})

9

	X	Y	Z
C	4.134058	5.019032	0.000000
C	2.915214	4.283392	0.000000
N	2.876251	2.956000	0.000000
C	4.014780	2.272451	0.000000
C	5.291871	2.901567	0.000000
C	5.316245	4.290169	0.000000
N	1.676909	4.905838	0.000000
N	3.870530	0.894035	0.000000
C	6.482778	2.069063	0.000000
H	6.266208	4.809600	0.000000
C	4.075887	6.470907	0.000000
C	1.646420	6.191545	0.000000
C	2.800063	7.058856	0.000000
C	4.936484	0.174512	0.000000
C	6.289238	0.677678	0.000000
C	7.799331	2.562234	0.000000
C	7.389651	–0.194765	0.000000
C	5.201578	7.313135	0.000000
C	2.659431	8.456100	0.000000
H	4.798901	–0.907257	0.000000
H	0.661454	6.659513	0.000000
H	7.214980	–1.265793	0.000000
C	8.671110	0.307181	0.000000
C	8.870799	1.694998	0.000000
H	7.986858	3.629044	0.000000
H	9.879936	2.091281	0.000000
H	9.522788	–0.362729	0.000000
C	5.049709	8.683199	0.000000
H	1.663492	8.887047	0.000000
C	3.773571	9.264047	0.000000
H	6.200905	6.895286	0.000000
H	5.927930	9.318908	0.000000
H	3.669212	10.342584	0.000000

Sum of electronic and thermal free energy: –894.611951 a.u.

N_{Im}= 0

10

	X	Y	Z
O	1.233591	2.028629	0.000000
C	0.035721	1.399700	0.000000
C	2.493941	1.404480	0.000000
O	–0.993025	2.003904	0.000000
N	0.102825	0.016133	0.000000
C	1.282013	–0.679798	0.000000
C	2.462610	–0.047190	0.000000
O	3.453368	2.108226	0.000000
H	–0.785825	–0.457599	0.000000
H	3.403171	–0.575139	0.000000
H	1.191699	–1.758494	0.000000

Sum of electronic and thermal free energy: –434.606097 a.u.
N_{Im}= 0

11

	X	Y	Z
N	1.261290	2.046881	0.000000
C	0.057614	1.372127	0.000000
C	2.465432	1.372958	0.000000
N	–1.056838	2.173404	0.000000
C	0.033561	0.017447	0.000000
C	1.262261	–0.764102	0.000000
C	2.490421	0.018295	0.000000
N	3.579329	2.175005	0.000000
H	1.260942	3.052402	0.000000
H	4.487305	1.750692	0.000000
H	3.527816	3.175638	0.000000
H	–1.964520	1.748462	0.000000
H	–1.006016	3.174071	0.000000
O	1.262686	–1.993408	0.000000
H	–0.910355	–0.512092	0.000000
H	3.434702	–0.510591	0.000000

Sum of electronic and thermal free energy: –434.108605 a.u.
N_{Im}= 3 (484*i* cm^{-1}, 479*i* cm^{-1}, 123*i* cm^{-1})

12

	X	Y	Z
C	3.872908	–1.429962	0.000000
C	2.770956	–2.248084	0.000000
N	1.494412	–1.739437	0.000000
C	1.289121	–0.380710	0.000000
C	2.336226	0.506530	0.000000
C	3.723252	0.029235	0.000000
N	2.912700	–3.598710	0.000000
N	0.006028	0.064210	0.000000
C	2.017010	1.899711	0.000000

O	4.679534	0.788082	0.000000
C	5.157119	–2.057381	0.000000
C	4.151678	–4.281738	0.000000
C	5.303270	–3.401384	0.000000
C	–0.377619	1.425978	0.000000
C	0.741369	2.347418	0.000000
H	2.854549	2.588687	0.000000
H	0.495538	3.400486	0.000000
H	6.018376	–1.398295	0.000000
H	6.272937	–3.880059	0.000000
O	–1.559077	1.700094	0.000000
O	4.150179	–5.494577	0.000000
H	–0.774450	–0.578321	0.000000
H	0.705267	–2.365655	0.000000
H	2.109636	–4.212780	0.000000

Sum of electronic and thermal free energy: –813.169798 a.u.
N_{Im}= 0

13

	X	Y	Z
O	1.173201	–0.652307	0.000000
C	0.002115	–0.011634	0.000000
C	2.436691	–0.023596	0.000000
N	–1.063232	–0.744999	0.000000
N	0.037639	1.347965	0.000000
C	1.212061	2.051822	0.000000
C	2.397079	1.426401	0.000000
O	3.393026	–0.729067	0.000000
H	–0.893949	1.776256	0.000000
H	3.335719	1.958315	0.000000
H	1.110139	3.129187	0.000000
C	–2.293971	–0.137536	0.000000
H	–3.116963	–0.863417	0.000000
O	–2.535935	1.063011	0.000000

Sum of electronic and thermal free energy: –528.020099 a.u.
N_{Im}= 0

14

	X	Y	Z
N	–2.014295	1.110325	0.000000
C	–2.758543	–0.126237	0.000000
N	–2.019621	–1.264690	0.000000
C	–0.704244	–1.211049	0.000000
C	0.047134	0.021624	0.000000
C	–0.690538	1.185137	0.000000
O	–3.963805	–0.036139	0.000000
N	–0.034598	–2.414424	0.000000
H	–0.237461	2.171207	0.000000
H	–2.587319	1.943188	0.000000
C	1.469222	–0.011117	0.000000

H	2.029178	0.918952	0.000000
C	2.085554	–1.217897	0.000000
H	3.163215	–1.315672	0.000000
C	1.264257	–2.390375	0.000000
H	1.754124	–3.362775	0.000000

Sum of electronic and thermal free energy: –509.097625 a.u.
N_{Im}= 0

15

	X	Y	Z
C	0.053293	1.335679	0.000000
N	0.054324	0.001508	0.000000
C	1.243656	–0.578579	0.000000
O	1.226061	–1.915257	0.000000
N	2.439635	0.001396	0.000000
C	2.414717	1.339154	0.000000
C	1.253367	2.074420	0.000000
N	–1.160498	1.936828	0.000000
H	3.381884	1.833237	0.000000
H	1.262618	3.156179	0.000000
H	–1.981810	1.357688	0.000000
H	–1.254070	2.934982	0.000000
H	2.146294	–2.197766	0.000000

Sum of electronic and thermal free energy: –394.844843 a.u.
N_{Im}= 1 (140*i* cm^{-1})

16

	X	Y	Z
C	–3.605944	–0.698128	0.000000
C	–4.836310	–1.524213	0.000000
C	–4.707741	–3.003905	0.000000
N	–3.630076	–3.671841	0.000000
C	–2.429603	–2.930370	0.000000
N	–2.487714	–1.518427	0.000000
O	–3.541678	0.501369	0.000000
N	–1.350120	–3.592323	0.000000
N	–6.064932	–1.181528	0.000000
C	–6.739485	–2.459438	0.000000
N	–6.015431	–3.517848	0.000000
H	–0.528604	–2.989541	0.000000
H	–7.821968	–2.472505	0.000000
H	–1.607283	–1.021611	0.000000

Sum of electronic and thermal free energy: –541.159552 a.u.
N_{Im}= 0

17

	X	Y	Z
C	0.271822	–1.386941	0.000000
C	–1.018519	–2.127244	0.000000
C	–2.317647	–1.359768	0.000000

N	–2.360927	–0.009364	0.000000
C	–1.208865	0.601531	0.000000
N	0.039700	–0.004865	0.000000
O	1.379346	–1.840211	0.000000
N	–1.196852	1.944283	0.000000
N	–1.209881	–3.375410	0.000000
C	–2.707615	–3.463121	0.000000
N	–3.307481	–2.180389	0.000000
H	–2.089823	2.408687	0.000000
H	–0.355529	2.492047	0.000000
O	–3.263228	–4.511383	0.000000
H	0.876392	0.562018	0.000000

Sum of electronic and thermal free energy: –616.429462 a.u.
N_{Im}= 0

18

	X	Y	Z
C	0.004634	0.005120	0.000000
N	1.257169	–0.651606	0.000000
C	2.444741	–0.004340	0.000000
C	2.479822	1.347595	0.000000
C	1.203446	1.986396	0.000000
N	0.055227	1.379855	0.000000
O	–1.006897	–0.654824	0.000000
O	1.208548	3.319260	0.000000
H	1.212002	–1.659049	0.000000
H	3.335270	–0.620395	0.000000
H	0.285450	3.601663	0.000000
H	3.398199	1.912966	0.000000

Sum of electronic and thermal free energy: –414.725776 a.u.
N_{Im}= 0

19

	X	Y	Z
C	–0.011502	–0.020168	0.000000
C	0.779857	1.161584	0.000000
N	2.087552	1.179528	0.000000
C	2.751696	–0.000461	0.000000
C	2.064193	–1.241020	0.000000
C	0.648998	–1.211668	0.000000
N	0.205422	2.439457	0.000000
N	4.105409	0.074443	0.000000
C	2.826845	–2.428310	0.000000
H	0.095474	–2.145120	0.000000
H	–1.088707	0.050478	0.000000
H	0.896261	3.177051	0.000000
C	–1.112867	2.805454	0.000000
H	–1.218399	3.904086	0.000000
O	–2.065133	2.063849	0.000000
H	2.323100	–3.389716	0.000000

C	4.190791	–2.337149	0.000000
H	4.820446	–3.218145	0.000000
C	4.776585	–1.050826	0.000000
H	5.860340	–0.959628	0.000000

Sum of electronic and thermal free energy: –586.502261 a.u.
N_{Im}= 0

20

	X	Y	Z
N	2.950225	–0.814394	0.000000
C	3.792249	0.311671	0.000000
C	3.349929	–2.117340	0.000000
O	3.285111	1.423879	0.000000
C	5.205629	0.007535	0.000000
C	5.595600	–1.300079	0.000000
C	4.692182	–2.389997	0.000000
N	2.363848	–3.064711	0.000000
H	1.967628	–0.578887	0.000000
C	6.153063	1.168740	0.000000
H	6.658685	–1.524298	0.000000
H	5.042144	–3.412791	0.000000
H	7.189681	0.825002	0.000000
H	5.993776	1.802895	0.876680
H	5.993776	1.802895	–0.876680
H	1.391194	–2.821752	0.000000
H	2.608190	–4.036738	0.000000

Sum of electronic and thermal free energy: –418.072079 a.u.
N_{Im}= 1 (409*i* cm^{-1})

21

	X	Y	Z
N	2.304137	1.395131	0.000000
C	2.425931	0.000290	0.000000
C	1.128755	2.097178	0.000000
O	3.538725	–0.501010	0.000000
C	1.161003	–0.713322	0.000000
C	0.003136	–0.000097	0.000000
C	–0.050672	1.422674	0.000000
N	1.290664	3.486958	0.000000
H	3.196002	1.870595	0.000000
C	1.229940	–2.208771	0.000000
H	–0.940749	–0.536908	0.000000
H	–0.985184	1.957852	0.000000
H	0.229718	–2.645692	0.000000
C	0.302590	4.442419	0.000000
H	2.234757	3.840581	0.000000
H	0.735779	5.457710	0.000000
O	–0.882231	4.235933	0.000000
H	1.774659	–2.570486	–0.876319
H	1.774659	–2.570486	0.876319

Sum of electronic and thermal free energy: –531.392348 a.u.
N_{Im}= 0

22

	X	Y	Z
N	–1.105728	0.785999	0.000000
C	0.000911	–0.002631	0.000000
N	–0.137417	–1.299591	0.000000
C	1.053275	–1.948934	0.000000
C	2.337093	–1.426975	0.000000
C	2.499500	–0.000595	0.000000
N	1.214553	0.627383	0.000000
O	3.491020	0.690555	0.000000
N	1.207112	–3.302706	0.000000
C	2.567277	–3.527817	0.000000
N	3.272278	–2.435258	0.000000
H	–2.000620	0.331106	0.000000
H	–1.060641	1.787273	0.000000
C	0.141442	–4.282296	0.000000
H	2.964466	–4.533142	0.000000
H	1.263295	1.636185	0.000000
H	0.583591	–5.278353	0.000000
H	–0.481522	–4.164296	0.887902
H	–0.481522	–4.164296	–0.887902

Sum of electronic and thermal free energy: –581.725583 a.u.
N_{Im}= 2 (336*i* cm^{-1}, 17*i* cm^{-1})

23

	X	Y	Z
C	0.058558	2.761490	0.000000
C	1.215120	1.932392	0.000000
N	1.203630	0.632747	0.000000
C	–0.000234	0.000370	0.000000
C	–1.219653	0.725797	0.000000
C	–1.151824	2.145218	0.000000
O	2.402970	2.557369	0.000000
N	0.032190	–1.351399	0.000000
C	–2.427137	0.001104	0.000000
H	–2.070287	2.723232	0.000000
H	0.172020	3.837293	0.000000
H	–3.372966	0.533783	0.000000
C	–2.379751	–1.367327	0.000000
H	–3.280425	–1.968376	0.000000
C	–1.114665	–1.990105	0.000000
H	–1.054303	–3.075946	0.000000
H	3.078169	1.869279	0.000000

Sum of electronic and thermal free energy: –493.060688 a.u.
N_{Im}= 0

24

	X	Y	Z
N	–0.041059	1.357591	0.000000
C	–1.212485	2.126063	0.000000
C	–0.002101	0.000193	0.000000
N	–1.045189	3.395013	0.000000
C	–2.456847	1.351828	0.000000
C	–2.399281	0.001858	0.000000
C	–1.166544	–0.730055	0.000000
N	1.218950	–0.611632	0.000000
C	1.308575	–1.985461	0.000000
H	2.060351	–0.060166	0.000000
C	–3.746961	2.114648	0.000000
H	–3.307738	–0.591904	0.000000
C	–1.134303	–2.192170	0.000000
H	–3.828040	2.757724	0.882996
H	–3.828040	2.757724	–0.882996
H	–4.597047	1.431785	0.000000
H	–1.934551	3.881822	0.000000
H	2.317109	–2.378222	0.000000
C	0.214464	–2.766069	0.000000
O	–2.147642	–2.879413	0.000000
H	0.310907	–3.843389	0.000000
H	0.805413	1.909001	0.000000

Sum of electronic and thermal free energy: –587.682155 a.u.
N_{Im}= 0

25

	X	Y	Z
C	0.182525	–1.455685	0.000000
C	1.475129	–2.034892	0.000000
N	2.633981	–1.291867	0.000000
C	2.490079	–0.002452	0.000000
C	1.269473	0.749088	0.000000
C	0.000902	–0.000600	0.000000
N	1.647969	–3.366815	0.000000
N	3.651614	0.753089	0.000000
C	1.311863	2.120953	0.000000
O	–1.088624	0.554660	0.000000
C	–0.925634	–2.305646	0.000000
C	0.584515	–4.157259	0.000000
C	0.859529	–5.635299	0.000000
C	–0.733216	–3.667228	0.000000
C	3.705725	2.102907	0.000000
C	5.067905	2.721536	0.000000
C	2.532370	2.817257	0.000000
H	–0.061625	–6.220521	0.000000
H	1.450152	–5.901766	–0.879671
H	1.450152	–5.901766	0.879671
H	4.993841	3.807896	0.000000
H	5.631279	2.412670	0.884916

H	5.631279	2.412670	–0.884916
H	0.366468	2.654403	0.000000
H	2.563865	3.897768	0.000000
H	–1.915711	–1.863068	0.000000
H	–1.570663	–4.354252	0.000000
H	4.503017	0.205057	0.000000

Sum of electronic and thermal free energy: –741.273789 a.u.
N_{Im}= 0

26

	X	Y	Z
N	–0.003731	0.003512	0.000000
C	–0.008371	–1.346429	0.000000
C	1.199665	0.743557	0.000000
N	–1.194376	–1.986589	0.000000
N	1.101659	–2.047189	0.000000
C	2.236141	–1.298082	0.000000
N	2.362006	–0.006789	0.000000
N	1.094729	2.009073	0.000000
H	3.157138	–1.876213	0.000000
H	2.024794	2.417391	0.000000
H	–0.851626	0.551444	0.000000
H	–1.174991	–2.991382	0.000000
H	–2.074556	–1.504874	0.000000

Sum of electronic and thermal free energy: –391.003421 a.u.
N_{Im}= 1 (166*i* cm^{-1})

27

	X	Y	Z
C	–0.117831	1.389778	0.000000
N	0.007266	–0.008905	0.000000
C	1.164829	–0.758795	0.000000
N	2.314841	0.015704	0.000000
C	2.304123	1.387681	0.000000
C	1.161137	2.090150	0.000000
O	–1.211432	1.905939	0.000000
O	1.188255	–1.965889	0.000000
H	3.278837	1.859004	0.000000
H	1.152849	3.169239	0.000000
H	–0.854958	–0.536628	0.000000
H	3.179914	–0.499880	0.000000

Sum of electronic and thermal free energy: –414.746469 a.u.
N_{Im}= 0

28

	X	Y	Z
N	3.669780	1.947127	0.000000
C	2.463719	1.343150	0.000000
N	2.406998	0.014120	0.000000
C	1.193939	–0.577742	0.000000

N	–0.007070	0.008005	0.000000
C	0.098083	1.335668	0.000000
C	1.266849	2.082853	0.000000
N	1.210745	–1.936829	0.000000
N	1.000243	3.439845	0.000000
C	–0.297795	3.507239	0.000000
N	–0.905585	2.268752	0.000000
H	0.343423	–2.439916	0.000000
H	2.090599	–2.417195	0.000000
H	3.729038	2.949680	0.000000
H	4.501399	1.384284	0.000000
H	–0.876775	4.419022	0.000000
H	–1.892272	2.073397	0.000000

Sum of electronic and thermal free energy: –522.568807 a.u.
N_{Im}= 1 (250*i* cm^{-1})

29

	X	Y	Z
N	–1.528306	–1.750004	0.000000
C	–0.247745	–1.354729	0.000000
N	0.006805	–0.032250	0.000000
C	1.280029	0.339366	0.000000
C	2.438699	–0.512137	0.000000
C	2.134411	–1.905786	0.000000
C	0.791834	–2.308465	0.000000
N	1.512549	1.684119	0.000000
H	0.680545	2.259956	0.000000
H	–1.728898	–2.736605	0.000000
H	–2.267444	–1.069979	0.000000
C	3.695966	0.063261	0.000000
C	2.738241	2.249162	0.000000
H	2.767648	3.329849	0.000000
C	3.854297	1.455315	0.000000
H	4.834836	1.910390	0.000000
H	4.558346	–0.593995	0.000000
N	0.727032	–3.664448	0.000000
N	2.924969	–2.991214	0.000000
C	2.021995	–3.999682	0.000000
H	2.339660	–5.034705	0.000000

Sum of electronic and thermal free energy: –620.765814 a.u.
N_{Im}= 0

30

	X	Y	Z
C	0.113772	1.743955	0.000000
O	0.088950	2.949225	0.000000
N	–1.066825	0.994255	0.000000
C	–1.224908	–0.377185	0.000000
O	–2.305415	–0.919364	0.000000
N	–0.031614	–1.085730	0.000000

C	1.181630	–0.446331	0.000000
C	1.304440	0.892591	0.000000
C	–0.130480	–2.541877	0.000000
H	2.052616	–1.088928	0.000000
Cl	2.853828	1.654052	0.000000
H	–1.926894	1.525792	0.000000
H	0.875082	–2.959349	0.000000
H	–0.668335	–2.881663	0.885437
H	–0.668335	–2.881663	–0.885437

Sum of electronic and thermal free energy: –913.638128 a.u.
N_{Im}= 0

31

	X	Y	Z
C	0.002020	0.001198	0.000000
N	1.106213	–0.750976	0.000000
C	2.207489	0.000725	0.000000
C	2.276637	1.386366	0.000000
C	1.040554	2.057348	0.000000
N	–0.085519	1.347834	0.000000
N	3.587216	1.822207	0.000000
C	4.280695	0.720635	0.000000
N	3.509615	–0.422654	0.000000
N	–1.187410	–0.658202	0.000000
N	0.964187	3.404393	0.000000
H	–1.194552	–1.660765	0.000000
H	–2.040640	–0.132061	0.000000
H	1.804551	3.954255	0.000000
H	0.062252	3.845745	0.000000
C	3.954653	–1.798903	0.000000
H	5.360227	0.660638	0.000000
H	5.044582	–1.816585	0.000000
H	3.584990	–2.315539	0.887312
H	3.584990	–2.315539	–0.887312

Sum of electronic and thermal free energy: –561.853242 a.u.
N_{Im}= 1 (258*i* cm^{-1})

32

	X	Y	Z
C	–1.118956	–2.135480	0.000000
N	–2.281969	–1.394820	0.000000
C	–2.423493	–0.000232	0.000000
C	–1.148883	0.698739	0.000000
C	–0.003044	–0.002849	0.000000
N	0.043747	–1.374241	0.000000
O	–1.102397	–3.345363	0.000000
O	–3.522542	0.507083	0.000000
C	1.305523	–2.105087	0.000000
H	0.963110	0.486902	0.000000
H	–1.152546	1.777930	0.000000

H	–3.136581	–1.934642	0.000000
H	2.123629	–1.386248	0.000000
H	1.375166	–2.738401	0.884987
H	1.375166	–2.738401	–0.884987

Sum of electronic and thermal free energy: –454.027231 a.u.
N_{Im}= 0

33

	X	Y	Z
O	–0.837543	–2.847537	0.000000
C	–1.602999	–1.915001	0.000000
N	–1.268181	–0.589705	0.000000
C	0.002916	0.000848	0.000000
C	1.179588	–0.726645	0.000000
C	2.372409	–0.000100	0.000000
C	2.351282	1.393297	0.000000
C	1.096726	1.995527	0.000000
N	–0.054475	1.335866	0.000000
N	0.927596	3.388256	0.000000
C	1.874325	4.372600	0.000000
O	3.072246	4.217431	0.000000
O	3.499587	–0.725546	0.000000
H	–0.041170	3.671960	0.000000
H	–2.021150	0.082381	0.000000
C	4.744273	–0.046471	0.000000
H	5.504385	–0.824810	0.000000
H	4.855568	0.574352	–0.894127
H	4.855568	0.574352	0.894127
H	–2.699442	–2.047227	0.000000
H	1.408030	5.373222	0.000000
H	1.183587	–1.805266	0.000000
H	3.238543	2.004304	0.000000

Sum of electronic and thermal free energy: –700.047861 a.u.
N_{Im}= 0

34

	X	Y	Z
O	–1.094548	–1.987363	0.000000
C	–1.161578	–0.776648	0.000000
N	–0.001145	0.000053	0.000000
C	0.104998	1.375898	0.000000
O	1.167323	1.957979	0.000000
N	–1.111755	2.034510	0.000000
C	–2.303402	1.343108	0.000000
C	–2.398895	0.001632	0.000000
C	–1.069154	3.491512	0.000000
H	–3.188495	1.968848	0.000000
C	–3.698780	–0.740790	0.000000
H	0.876496	–0.501226	0.000000
H	–2.090385	3.869778	0.000000

H	–0.545185	3.854797	0.884887
H	–0.545185	3.854797	–0.884887
H	–4.545018	–0.050858	0.000000
H	–3.773420	–1.387543	–0.877642
H	–3.773420	–1.387543	0.877642

Sum of electronic and thermal free energy: –493.319097 a.u.
N_{Im}= 0

35

	X	Y	Z
O	–0.897094	–4.155125	0.000000
C	–1.640105	–3.204470	0.000000
N	–1.272456	–1.887446	0.000000
C	0.014307	–1.331513	0.000000
N	0.002498	–0.001457	0.000000
C	1.166015	0.643072	0.000000
C	2.401239	–0.001556	0.000000
C	2.380144	–1.388256	0.000000
C	1.183523	–2.089312	0.000000
N	1.016415	2.036787	0.000000
C	1.981774	3.005186	0.000000
O	3.175037	2.826479	0.000000
H	0.053038	2.338272	0.000000
H	–2.009160	–1.197333	0.000000
H	–2.739142	–3.310191	0.000000
H	1.140687	–3.167264	0.000000
H	3.318418	0.566422	0.000000
H	1.532723	4.013855	0.000000
H	3.316529	–1.934418	0.000000

Sum of electronic and thermal free energy: –585.552176 a.u.
N_{Im}= 0

36

	X	Y	Z
O	0.722240	2.317734	0.000000
C	1.484313	1.228211	0.000000
C	2.879528	1.322386	0.000000
C	3.538758	0.092162	0.000000
N	2.989758	–1.119405	0.000000
C	1.658092	–1.064014	0.000000
N	0.890155	0.048720	0.000000
N	0.985472	–2.242723	0.000000
N	3.781282	2.371690	0.000000
C	4.941360	1.791905	0.000000
N	4.867626	0.412569	0.000000
H	5.631592	–0.241845	0.000000
H	5.893226	2.302831	0.000000
H	–0.193748	2.017690	0.000000
H	1.500698	–3.103171	0.000000
H	–0.017081	–2.240079	0.000000

Sum of electronic and thermal free energy: –542.441172 a.u.
N_{Im}= 1 (219*i* cm^{-1})

37

	X	Y	Z
C	–4.298676	0.768262	0.000000
C	–3.139719	–0.130606	0.000000
N	–1.913512	0.521282	0.000000
C	–1.725659	1.880948	0.000000
C	–2.854763	2.720873	0.000000
C	–4.158451	2.105528	0.000000
O	–3.205498	–1.343638	0.000000
N	–0.466910	2.317339	0.000000
C	–2.621637	4.096117	0.000000
H	–5.032271	2.749837	0.000000
H	–5.267619	0.286511	0.000000
H	–3.462471	4.782048	0.000000
C	–1.320865	4.564394	0.000000
H	–1.101228	5.624072	0.000000
C	–0.283449	3.631352	0.000000
H	–1.085891	–0.060129	0.000000
H	0.750620	3.963059	0.000000

Sum of electronic and thermal free energy: –493.075414 a.u.
N_{Im}= 0

38

	X	Y	Z
N	–0.634311	1.179443	0.000000
C	–1.961274	1.180367	0.000000
C	–0.017131	–0.004469	0.000000
N	–2.560401	2.403119	0.000000
C	–2.752418	–0.006956	0.000000
C	–2.073174	–1.197369	0.000000
C	–0.669660	–1.237636	0.000000
N	1.357165	0.026289	0.000000
C	2.094337	–1.122132	0.000000
H	1.794606	0.933330	0.000000
C	–4.252455	0.074003	0.000000
H	–2.602698	–2.144896	0.000000
C	0.075754	–2.507495	0.000000
H	–4.689586	–0.925049	0.000000
H	–3.556916	2.507077	0.000000
H	–1.978215	3.221357	0.000000
H	3.168285	–0.981623	0.000000
C	1.525921	–2.346779	0.000000
O	–0.482451	–3.597924	0.000000
H	2.141674	–3.235946	0.000000
H	–4.628896	0.598765	0.885626
H	–4.628896	0.598765	–0.885626

Sum of electronic and thermal free energy: –587.712215 a.u.

N_{Im}= 1 (271*i* cm^{-1})

39

	X	Y	Z
N	1.215161	0.477803	0.000000
C	–0.001368	–0.002348	0.000000
C	–1.280030	0.690004	0.000000
C	–2.439249	–0.002196	0.000000
C	–2.463592	–1.436848	0.000000
C	–1.230530	–2.110837	0.000000
N	–0.079494	–1.370142	0.000000
C	–3.617614	–2.226256	0.000000
C	–3.493906	–3.600418	0.000000
C	–2.208780	–4.152758	0.000000
N	–1.094222	–3.437672	0.000000
C	1.461432	1.833311	0.000000
O	0.670233	2.756452	0.000000
H	–3.384803	0.530970	0.000000
H	–1.250412	1.768460	0.000000
H	2.545385	2.033307	0.000000
H	–4.592791	–1.750810	0.000000
H	–4.362309	–4.246209	0.000000
H	–2.078352	–5.230815	0.000000
H	0.801330	–1.869511	0.000000

Sum of electronic and thermal free energy: –586.489840 a.u.
N_{Im}= 1 (31*i* cm^{-1})

40

	X	Y	Z
N	–1.276576	–0.573473	0.000000
C	0.002939	0.001414	0.000000
C	1.183662	–0.725784	0.000000
C	2.371592	0.002346	0.000000
C	2.381004	1.386509	0.000000
C	1.116642	1.990651	0.000000
N	–0.029262	1.337449	0.000000
O	1.057440	3.337353	0.000000
C	–1.622538	–1.894580	0.000000
O	–0.864104	–2.833920	0.000000
C	3.632673	2.213987	0.000000
H	3.316353	–0.532006	0.000000
H	1.168149	–1.804337	0.000000
H	4.516758	1.573927	0.000000
H	3.675459	2.862962	–0.878752
H	3.675459	2.862962	0.878752
H	–2.023971	0.104770	0.000000
H	–2.719893	–2.018562	0.000000
H	0.126141	3.579463	0.000000

Sum of electronic and thermal free energy: –531.400500 a.u.
N_{Im}= 0

41

	X	Y	Z
C	1.122500	2.123359	0.000000
C	–0.061763	1.369269	0.000000
N	0.000003	0.000004	0.000000
C	1.181577	–0.694678	0.000000
C	2.401801	–0.000284	0.000000
C	2.444318	1.472481	0.000000
N	–1.284848	1.901888	0.000000
N	1.080672	–2.024881	0.000000
C	3.565066	–0.769188	0.000000
O	3.489332	2.102007	0.000000
H	–0.864698	–0.520899	0.000000
C	0.986562	3.511134	0.000000
C	–1.392160	3.227079	0.000000
C	–2.788468	3.778612	0.000000
C	–0.272469	4.072811	0.000000
C	2.201993	–2.739223	0.000000
C	2.036833	–4.231399	0.000000
C	3.473045	–2.144751	0.000000
H	–2.791700	4.869339	0.000000
H	–3.328752	3.422223	–0.880191
H	–3.328752	3.422223	0.880191
H	2.999539	–4.744130	0.000000
H	1.469218	–4.542418	0.880191
H	1.469218	–4.542418	–0.880191
H	4.520175	–0.255909	0.000000
H	4.360530	–2.764997	0.000000
H	1.886786	4.115524	0.000000
H	–0.405909	5.147301	0.000000

Sum of electronic and thermal free energy: –741.300654 a.u.
N_{Im}= 0

42

	X	Y	Z
N	–0.001729	–0.000993	0.000000
C	–1.187588	0.611124	0.000000
N	–2.386111	–0.001065	0.000000
C	–2.305909	–1.323231	0.000000
N	–1.204845	–2.059582	0.000000
C	–0.071572	–1.333685	0.000000
N	1.090701	–2.016716	0.000000
N	–1.190870	1.959234	0.000000
H	1.960578	–1.516210	0.000000
H	–0.319842	2.457734	0.000000
H	–3.248909	–1.864365	0.000000
H	1.067880	–3.020180	0.000000
H	–2.068755	2.445834	0.000000

Sum of electronic and thermal free energy: –391.036194 a.u.

N_{Im}= 0

43

	X	Y	Z
O	0.979880	–0.703806	0.000000
C	–0.055980	–0.078067	0.000000
N	–0.007891	1.332918	0.000000
C	–1.109402	2.114561	0.000000
C	–2.346031	1.563648	0.000000
C	–2.373692	0.135210	0.000000
N	–1.311606	–0.629521	0.000000
N	–3.558620	–0.579730	0.000000
H	–3.248217	2.150825	0.000000
H	–0.946336	3.185233	0.000000
H	0.918118	1.732620	0.000000
H	–3.389346	–1.575612	0.000000
C	–4.867588	–0.105249	0.000000
N	–5.797510	–1.104388	0.000000
O	–5.167928	1.068387	0.000000
H	–6.762679	–0.826376	0.000000
H	–5.572433	–2.082643	0.000000

Sum of electronic and thermal free energy: –563.531476 a.u.
N_{Im}= 1 (205*i* cm^{-1})

44

	X	Y	Z
O	2.203668	4.014897	0.000000
C	2.173543	2.807183	0.000000
N	3.411101	2.098233	0.000000
C	3.511871	0.763213	0.000000
C	2.382691	0.000267	0.000000
C	1.161879	0.733033	0.000000
N	1.043435	2.034902	0.000000
N	–0.001922	0.006970	0.000000
C	–0.025508	–1.371672	0.000000
C	1.125388	–2.107354	0.000000
N	–1.269569	–1.921343	0.000000
H	–0.852484	0.550372	0.000000
C	2.422290	–1.481404	0.000000
H	4.497380	0.311355	0.000000
H	4.233873	2.683470	0.000000
O	3.488034	–2.084350	0.000000
H	1.075587	–3.187942	0.000000
H	–1.369317	–2.919443	0.000000
H	–2.103490	–1.363838	0.000000

Sum of electronic and thermal free energy: –639.706254 a.u.
N_{Im}= 1 (336*i* cm^{-1})

45

	X	Y	Z

H	0.156348	–2.331727	0.000000
N	1.105085	–1.988054	0.000000
C	1.143784	–0.599779	0.000000
N	0.003809	0.000585	0.000000
C	0.026239	1.378314	0.000000
C	1.234180	2.101958	0.000000
C	2.514902	1.389398	0.000000
N	2.363164	0.002773	0.000000
O	3.613359	1.897743	0.000000
C	1.194838	3.495834	0.000000
N	–1.167339	1.990406	0.000000
C	2.178061	–2.867287	0.000000
O	3.339209	–2.501975	0.000000
N	1.820300	–4.178355	0.000000
H	2.564577	–4.853379	0.000000
H	0.869275	–4.499853	0.000000
H	3.192993	–0.588933	0.000000
H	2.128189	4.047170	0.000000
C	–0.033998	4.118966	0.000000
C	–1.178153	3.312612	0.000000
H	–2.162458	3.774260	0.000000
H	–0.125313	5.197624	0.000000

Sum of electronic and thermal free energy: –733.175521 a.u.

N_{Im}= 1 (155*i* cm^{-1})

46

	X	Y	Z
N	0.005214	–0.000477	0.000000
C	1.156106	0.592522	0.000000
N	2.369446	–0.001784	0.000000
C	2.448432	–1.382100	0.000000
C	1.255086	–2.104974	0.000000
C	–0.049121	–1.389091	0.000000
N	3.664243	–1.918986	0.000000
O	–1.101551	–1.989884	0.000000
N	1.117613	1.979843	0.000000
H	0.168102	2.321744	0.000000
C	2.192431	2.857601	0.000000
N	1.837667	4.168901	0.000000
O	3.352638	2.488615	0.000000
H	0.886995	4.491620	0.000000
H	3.209019	0.574020	0.000000
H	2.582866	4.842925	0.000000
C	1.349754	–3.493006	0.000000
H	0.435427	–4.075247	0.000000
C	2.603642	–4.077593	0.000000
H	2.726133	–5.153130	0.000000
C	3.723739	–3.245860	0.000000
H	4.722681	–3.671831	0.000000

Sum of electronic and thermal free energy: –733.172342 a.u.

N_{Im}= 1 (139*i* cm^{-1})

47

	X	Y	Z
N	–1.412616	–1.135001	0.000000
C	–2.607834	–1.672539	0.000000
C	–2.865455	–3.068933	0.000000
C	–1.784141	–3.900963	0.000000
C	–0.476978	–3.366314	0.000000
C	–0.338701	–1.956256	0.000000
N	0.874292	–1.359265	0.000000
C	1.942318	–2.118748	0.000000
C	1.923767	–3.538585	0.000000
C	0.701421	–4.144708	0.000000
N	3.139031	–1.391189	0.000000
C	4.433064	–1.836996	0.000000
O	4.797081	–2.987391	0.000000
N	–3.640414	–0.726365	0.000000
C	–4.996399	–0.912297	0.000000
O	–5.576963	–1.970059	0.000000
H	2.988696	–0.391970	0.000000
H	–3.298834	0.224614	0.000000
H	–3.881942	–3.431869	0.000000
H	–1.921462	–4.977383	0.000000
H	0.627021	–5.227298	0.000000
H	2.850386	–4.092071	0.000000
H	5.142552	–0.991486	0.000000
H	–5.528119	0.054933	0.000000

Sum of electronic and thermal free energy: –755.183619 a.u.
N_{Im}= 0

48

	X	Y	Z
O	–3.618992	1.883750	0.000000
C	–1.238250	2.120533	0.000000
C	–0.083518	1.414040	0.000000
H	0.872162	1.927606	0.000000
N	0.006574	0.049161	0.000000
C	–1.119450	–0.608430	0.000000
N	–2.329139	0.016129	0.000000
C	–2.500109	1.419597	0.000000
N	–1.153985	–1.975499	0.000000
C	–0.101794	–2.934057	0.000000
O	–0.411067	–4.108046	0.000000
N	1.148323	–2.451042	0.000000
C	2.278048	–3.357763	0.000000
H	3.192463	–2.765495	0.000000
H	–2.050489	–2.437346	0.000000
H	–3.191085	–0.512574	0.000000
H	1.263600	–1.442994	0.000000

H	–1.254747	3.200746	0.000000
H	2.267328	–3.997879	0.885068
H	2.267328	–3.997879	–0.885068

Sum of electronic and thermal free energy: –602.814294 a.u.
N_{Im}= 0

49

	X	Y	Z
O	–4.375708	–2.548826	0.000000
C	–5.367289	–1.849007	0.000000
C	–6.748159	–2.290979	0.000000
C	–7.769043	–1.402533	0.000000
C	–7.551226	0.008605	0.000000
C	–6.238690	0.448214	0.000000
N	–5.216251	–0.445043	0.000000
N	–5.960513	1.777089	0.000000
C	–6.926687	2.806863	0.000000
H	–5.004491	2.106348	0.000000
H	–4.254774	–0.132071	0.000000
H	–6.909815	–3.360005	0.000000
H	–8.794267	–1.759733	0.000000
O	–6.556636	3.962736	0.000000
C	–8.295195	2.327981	0.000000
H	–9.068112	3.083990	0.000000
C	–8.575028	1.003885	0.000000
H	–9.608576	0.671537	0.000000

Sum of electronic and thermal free energy: –568.307769 a.u.
N_{Im}= 0

50

	X	Y	Z
N	–3.181949	1.702852	0.000000
C	–3.186039	0.335630	0.000000
C	–4.385224	–0.393988	0.000000
C	–4.294515	–1.771703	0.000000
C	–3.058975	–2.410765	0.000000
C	–1.936847	–1.588364	0.000000
N	–1.991737	–0.254371	0.000000
N	–0.618964	–2.055599	0.000000
C	–0.170304	–3.361781	0.000000
O	–0.891545	–4.337641	0.000000
N	1.197251	–3.467603	0.000000
H	1.578491	–4.396256	0.000000
H	1.822583	–2.682945	0.000000
H	0.049906	–1.301105	0.000000
H	–2.956456	–3.483819	0.000000
H	–5.199829	–2.369043	0.000000
H	–5.342438	0.112966	0.000000
H	–4.034544	2.228846	0.000000
H	–2.301225	2.183628	0.000000

Sum of electronic and thermal free energy: –527.591876 a.u.
N_{Im}= 2 (333*i* cm^{-1}, 297*i* cm^{-1})

51

	X	Y	Z
O	1.062660	2.013323	0.000000
C	1.118157	0.806609	0.000000
N	2.387213	0.178763	0.000000
C	2.545876	–1.157748	0.000000
C	1.469559	–1.981227	0.000000
C	0.190249	–1.336847	0.000000
N	0.038090	–0.036866	0.000000
N	–1.015188	–2.016947	0.000000
C	–1.422049	–3.349269	0.000000
O	–2.608991	–3.576505	0.000000
H	1.608927	–3.046208	0.000000
H	3.563087	–1.529760	0.000000
H	3.179917	0.802717	0.000000
H	–1.801897	–1.377451	0.000000
C	–0.402684	–4.458815	0.000000
H	–0.949714	–5.398876	0.000000
H	0.230040	–4.412127	–0.889017
H	0.230040	–4.412127	0.889017

Sum of electronic and thermal free energy: –547.452978 a.u.
N_{Im}= 1 (28*i* cm^{-1})

52

	X	Y	Z
N	–3.252521	–1.762361	0.000000
C	–3.128266	–0.405744	0.000000
C	–4.272138	0.426635	0.000000
C	–4.086389	1.785563	0.000000
C	–2.792739	2.320769	0.000000
C	–1.747131	1.401300	0.000000
N	–1.887818	0.074684	0.000000
N	–0.446770	1.861334	0.000000
C	–0.147877	3.198356	0.000000
C	–1.137190	4.139712	0.000000
N	1.184594	3.501190	0.000000
H	1.895341	2.794232	0.000000
H	0.273404	1.156385	0.000000
C	–2.533948	3.777033	0.000000
H	–4.921978	2.476729	0.000000
H	–5.263632	–0.009888	0.000000
O	–3.452214	4.591542	0.000000
H	–0.881348	5.191288	0.000000
H	1.471936	4.461581	0.000000
H	–2.421643	–2.325691	0.000000
H	–4.151453	–2.205379	0.000000

Sum of electronic and thermal free energy: –603.770304 a.u.

N_{Im}= 2 (409*i* cm^{-1}, 273*i* cm^{-1})

53

	X	Y	Z
O	–2.207761	4.013431	0.000000
C	–2.179770	2.807058	0.000000
N	–3.422987	2.105001	0.000000
C	–3.531282	0.769023	0.000000
C	–2.405771	–0.001349	0.000000
C	–1.167007	0.729298	0.000000
N	–1.053811	2.029841	0.000000
N	–0.018590	–0.009949	0.000000
C	0.069726	–1.405506	0.000000
C	–1.218215	–2.110770	0.000000
O	1.150637	–1.949678	0.000000
H	0.855162	0.501140	0.000000
C	–2.381178	–1.441406	0.000000
H	–4.530760	0.348849	0.000000
H	–4.241829	2.695357	0.000000
H	–1.164927	–3.190893	0.000000
H	–3.326206	–1.975686	0.000000

Sum of electronic and thermal free energy: –584.364623 a.u.
N_{Im}= 0

54

	X	Y	Z
N	2.437915	–2.502092	0.000000
C	1.193095	–1.967229	0.000000
C	0.025454	–2.782267	0.000000
C	–1.230601	–2.144733	0.000000
C	–1.285535	–0.779245	0.000000
C	–0.056600	–0.063664	0.000000
N	1.126720	–0.614718	0.000000
N	–0.110731	1.316680	0.000000
C	–1.261655	2.071840	0.000000
C	–2.572020	–0.053999	0.000000
H	–2.153426	–2.715821	0.000000
C	0.184770	–4.186775	0.000000
H	0.764372	1.820712	0.000000
O	–1.263968	3.277050	0.000000
N	–2.436878	1.325643	0.000000
O	–3.657334	–0.585726	0.000000
H	–3.289987	1.867775	0.000000
H	–0.692980	–4.824628	0.000000
C	1.447198	–4.706099	0.000000
H	1.624791	–5.774031	0.000000
C	2.540472	–3.808063	0.000000
H	3.553037	–4.204780	0.000000

Sum of electronic and thermal free energy: –754.020277 a.u.
N_{Im}= 0

55

	X	Y	Z
N	2.344260	1.332951	0.000000
C	2.252202	0.000056	0.000000
N	1.130402	–0.710650	0.000000
C	0.002638	0.000536	0.000000
C	–0.043305	1.381113	0.000000
C	1.203048	2.011605	0.000000
H	–0.918616	–0.574457	0.000000
H	–0.966720	1.937117	0.000000
N	1.380150	3.391736	0.000000
H	2.349734	3.675617	0.000000
C	0.424905	4.378738	0.000000
O	–0.767401	4.211363	0.000000
N	3.478549	–0.637344	0.000000
H	4.268417	–0.006670	0.000000
C	3.859609	–1.980265	0.000000
O	5.045435	–2.223183	0.000000
H	0.887776	5.380237	0.000000
C	2.807992	–3.052708	0.000000
H	2.161504	–2.961017	0.873501
H	2.161502	–2.960998	–0.873501
H	3.321437	–4.012288	0.000000

Sum of electronic and thermal free energy: –640.902401 a.u.
N_{Im}= 0

56

	X	Y	Z
H	4.374226	–0.940824	0.000000
N	5.374541	–1.068323	0.000000
C	6.109376	0.090422	0.000000
N	5.378043	1.209029	0.000000
C	6.037440	2.361795	0.000000
C	7.435771	2.424877	0.000000
C	8.075090	1.203464	0.000000
N	7.442152	0.028356	0.000000
H	9.159753	1.155961	0.000000
H	7.964429	3.363550	0.000000
C	5.745035	–2.429666	0.000000
O	4.864297	–3.269070	0.000000
N	7.063415	–2.699481	0.000000
H	7.705900	–1.916256	0.000000
C	7.524015	–4.071199	0.000000
H	7.169652	–4.606148	0.884484
H	7.169652	–4.606148	–0.884484
H	8.613926	–4.067769	0.000000
N	5.202699	3.470358	0.000000
H	4.223145	3.224593	0.000000
C	5.541075	4.812971	0.000000

O	6.682331	5.210297	0.000000
C	4.340694	5.731778	0.000000
H	3.723338	5.557616	0.885213
H	3.723338	5.557616	–0.885213
H	4.689800	6.761713	0.000000

Sum of electronic and thermal free energy: –735.554076 a.u.
N_{Im}= 1 (1*i* cm^{-1})

57

	X	Y	Z
N	0.632919	1.811157	0.000000
C	0.544050	3.126157	0.000000
C	1.657423	3.971354	0.000000
C	2.887877	3.347763	0.000000
N	3.003909	2.007978	0.000000
C	1.876142	1.305112	0.000000
N	1.926093	–0.065188	0.000000
C	3.004009	–0.975811	0.000000
O	2.756627	–2.166897	0.000000
N	4.241716	–0.447420	0.000000
C	5.400994	–1.313008	0.000000
H	6.295479	–0.690103	0.000000
H	5.414188	–1.954732	0.884380
H	5.414188	–1.954732	–0.884380
H	4.321142	0.562953	0.000000
H	1.029601	–0.527066	0.000000
C	4.171871	4.119558	0.000000
H	1.543256	5.045605	0.000000
O	–0.676862	3.664807	0.000000
H	–1.311025	2.939002	0.000000
H	3.995510	5.195453	0.000000
H	4.761327	3.855275	0.881300
H	4.761327	3.855275	–0.881300

Sum of electronic and thermal free energy: –642.112359 a.u.
N_{Im}= 0

58

	X	Y	Z
N	0.031462	–1.335611	0.000000
C	–1.161346	–1.930959	0.000000
N	–2.342226	–1.293938	0.000000
C	–2.242906	0.033195	0.000000
N	–1.134304	0.744317	0.000000
C	–0.009838	–0.003104	0.000000
H	–3.178649	0.585716	0.000000
N	1.159996	0.658668	0.000000
H	2.022245	0.144085	0.000000
N	–1.129529	–3.294170	0.000000
H	–0.205569	–3.700137	0.000000
C	–2.152052	–4.273381	0.000000

O	–1.825539	–5.444027	0.000000
N	–3.419555	–3.825398	0.000000
H	–3.567592	–2.823066	0.000000
C	–4.521102	–4.764334	0.000000
H	–4.492252	–5.405031	–0.884601
H	–4.492252	–5.405031	0.884601
H	–5.453381	–4.199978	0.000000
H	1.155170	1.662792	0.000000

Sum of electronic and thermal free energy: –599.002802 a.u.
N_{Im}= 0

59

	X	Y	Z
H	–1.946410	–2.601589	0.000000
N	–2.867936	–3.018280	0.000000
C	–2.855810	–4.393298	0.000000
N	–1.634649	–4.925813	0.000000
C	–1.610682	–6.260488	0.000000
N	–2.698121	–7.056806	0.000000
C	–3.839568	–6.395501	0.000000
N	–4.003026	–5.074816	0.000000
H	–4.747887	–6.992243	0.000000
C	–3.895391	–2.068058	0.000000
O	–3.572152	–0.902821	0.000000
C	–5.327335	–2.519506	0.000000
N	–0.409192	–6.863659	0.000000
H	0.426676	–6.307346	0.000000
H	–0.364414	–7.866805	0.000000
H	–5.949977	–1.626904	0.000000
H	–5.538028	–3.137598	–0.873340
H	–5.538028	–3.137598	0.873340

Sum of electronic and thermal free energy: –543.647460 a.u.
N_{Im}= 1 (85*i* cm^{-1})

Table S11. Optimized Cartesian coordinates (in Å) and computed total electronic energies (including thermal free energy corrections) (in a.u.) for all monomers and complexes at IEF-PCM-ωB97XD/6-311+G(*d*,*p*) in implicit chloroform solvation. All geometries were optimized at C_s symmetry.

1. Triple hydrogen bonding monomers and complexes

AAA–DDD arrays

7•8

	X	Y	Z
C	4.086436	4.984856	0.000000
C	2.858786	4.252014	0.000000
N	2.807566	2.918444	0.000000
C	3.957912	2.241881	0.000000
C	5.237398	2.879923	0.000000
C	5.277710	4.269101	0.000000
N	1.653315	4.897420	0.000000
N	3.850712	0.878717	0.000000
C	6.402226	2.060399	0.000000
H	6.230221	4.789926	0.000000
N	0.037232	1.403627	0.000000
C	–1.120857	2.152476	0.000000
C	0.042690	0.024529	0.000000
N	–0.937375	3.479104	0.000000
C	–2.359029	1.531055	0.000000
C	–2.485180	0.024390	0.000000
C	–1.148671	–0.682503	0.000000
N	1.258570	–0.536938	0.000000
H	2.116383	0.015365	0.000000
H	–0.009471	3.903223	0.000000
H	–1.777436	4.043481	0.000000
H	1.280355	–1.548743	0.000000
C	4.025116	6.407770	0.000000
C	1.644668	6.202039	0.000000
C	2.810951	7.016409	0.000000
C	4.944376	0.167377	0.000000
C	6.259381	0.709757	0.000000
H	7.380116	2.528882	0.000000
H	7.111956	0.043654	0.000000
H	4.947257	6.978210	0.000000
H	2.710280	8.093648	0.000000
H	0.933309	1.893597	0.000000
C	–3.537086	2.332800	0.000000
C	–1.109458	–2.106959	0.000000
O	–4.684007	1.603559	0.000000
O	–3.618054	3.566233	0.000000
H	–5.408238	2.239089	0.000000
O	–2.342345	–2.678980	0.000000
O	–0.114753	–2.840768	0.000000

H	–2.198151	–3.631669	0.000000
H	4.815552	–0.911870	0.000000
H	0.666551	6.676020	0.000000
H	–3.070752	–0.295797	0.869867
H	–3.070752	–0.295797	–0.869867

Sum of electronic and thermal free energy: –1324.692856 a.u.
N_{Im}= 1 (13*i* cm^{-1})

9•8

	X	Y	Z
C	4.113159	5.007848	0.000000
C	2.897653	4.274761	0.000000
N	2.853052	2.943311	0.000000
C	3.998042	2.262320	0.000000
C	5.271179	2.890007	0.000000
C	5.295386	4.278762	0.000000
N	1.665269	4.898394	0.000000
N	3.857988	0.888249	0.000000
C	6.460542	2.055366	0.000000
H	6.244620	4.797797	0.000000
N	0.056540	1.414186	0.000000
C	–1.101899	2.162796	0.000000
C	0.061607	0.034920	0.000000
N	–0.918273	3.489040	0.000000
C	–2.340086	1.541227	0.000000
C	–2.466419	0.034651	0.000000
C	–1.129888	–0.672042	0.000000
N	1.277242	–0.526215	0.000000
H	2.133789	0.028716	0.000000
H	0.011160	3.910675	0.000000
H	–1.758069	4.053737	0.000000
H	1.299440	–1.537970	0.000000
C	4.052352	6.459575	0.000000
C	1.624856	6.188989	0.000000
C	2.775480	7.049469	0.000000
C	4.922704	0.157735	0.000000
C	6.268077	0.662049	0.000000
C	7.775452	2.550403	0.000000
C	7.367471	–0.213496	0.000000
C	5.178725	7.299415	0.000000
C	2.631683	8.447528	0.000000
H	0.952425	1.904049	0.000000
C	–3.517913	2.343150	0.000000
C	–1.090408	–2.096401	0.000000
O	–4.665055	1.614132	0.000000
O	–3.598819	3.576651	0.000000
H	–5.389054	2.249916	0.000000
O	–2.323230	–2.668721	0.000000
O	–0.095618	–2.830202	0.000000
H	–2.178702	–3.621353	0.000000

H	4.777429	–0.921347	0.000000
H	0.637999	6.649029	0.000000
H	–3.051979	–0.285528	0.869891
H	–3.051979	–0.285528	–0.869891
H	7.193695	–1.284102	0.000000
C	8.647350	0.291644	0.000000
C	8.845482	1.680349	0.000000
H	7.965602	3.616265	0.000000
H	9.854323	2.076487	0.000000
H	9.499956	–0.376457	0.000000
C	5.023704	8.669790	0.000000
H	1.636581	8.879000	0.000000
C	3.747657	9.252424	0.000000
H	6.178669	6.884289	0.000000
H	5.901642	9.305329	0.000000
H	3.645320	10.330767	0.000000

Sum of electronic and thermal free energy: –1631.865995 a.u.
N_{Im}= 1 (10*i* cm^{-1})

10•11

	X	Y	Z
N	1.173982	1.962275	0.000000
C	–0.039401	1.334237	0.000000
O	0.010616	–0.021647	0.000000
C	1.183046	–0.798383	0.000000
C	2.412792	–0.053473	0.000000
C	2.365242	1.288451	0.000000
O	–1.099788	1.897335	0.000000
O	1.026649	–1.986110	0.000000
H	3.251391	1.908106	0.000000
N	–2.800568	–1.521455	0.000000
C	–3.962528	–0.786057	0.000000
C	–2.811615	–2.896602	0.000000
N	–3.801275	0.564437	0.000000
C	–5.172028	–1.422887	0.000000
C	–5.261222	–2.863325	0.000000
C	–4.002127	–3.568443	0.000000
N	–1.588921	–3.491870	0.000000
H	–0.724813	–2.967937	0.000000
H	–2.892673	1.006520	0.000000
H	–4.615777	1.150334	0.000000
H	–1.536784	–4.493891	0.000000
H	–1.912413	–1.038258	0.000000
H	–4.006204	–4.651195	0.000000
H	–6.084417	–0.839811	0.000000
O	–6.358331	–3.461435	0.000000
H	3.344343	–0.596635	0.000000
H	1.152603	2.971609	0.000000

Sum of electronic and thermal free energy: –868.747838 a.u.
N_{Im}= 3 (240*i* cm^{-1}, 228*i* cm^{-1}, 12*i* cm^{-1})

10•8

	X	Y	Z
N	4.012008	4.899435	0.000000
C	2.799565	4.270016	0.000000
O	2.850539	2.914340	0.000000
C	4.023600	2.138991	0.000000
C	5.252725	2.884761	0.000000
C	5.203909	4.226669	0.000000
O	1.738209	4.831462	0.000000
O	3.867502	0.951166	0.000000
H	6.089472	4.847154	0.000000
N	0.026125	1.403295	0.000000
C	–1.129640	2.158076	0.000000
C	0.036177	0.022785	0.000000
N	–0.939339	3.486648	0.000000
C	–2.363144	1.537658	0.000000
C	–2.488645	0.030304	0.000000
C	–1.152764	–0.679174	0.000000
N	1.256861	–0.534974	0.000000
H	2.106068	0.014666	0.000000
H	–0.017601	3.903232	0.000000
H	–1.772655	4.061136	0.000000
H	1.290414	–1.546565	0.000000
H	0.913408	1.886768	0.000000
C	–3.543053	2.343013	0.000000
C	–1.113584	–2.107260	0.000000
O	–4.687770	1.615558	0.000000
O	–3.615559	3.574849	0.000000
H	–5.414357	2.248729	0.000000
O	–2.344729	–2.676506	0.000000
O	–0.116772	–2.834362	0.000000
H	–2.205197	–3.630115	0.000000
H	–3.073705	–0.289151	0.870073
H	–3.073705	–0.289151	–0.870073
H	3.989436	5.908778	0.000000
H	6.184692	2.342328	0.000000

Sum of electronic and thermal free energy: –1171.845158 a.u.
N_{Im}= 3 (42*i* cm^{-1}, 39*i* cm^{-1}, 12*i* cm^{-1})

10•12

	X	Y	Z
N	1.085750	1.923641	0.000000
C	–0.125103	1.297039	0.000000
O	–0.074029	–0.059925	0.000000
C	1.098313	–0.839493	0.000000
C	2.325871	–0.094820	0.000000
C	2.276555	1.247644	0.000000
O	–1.190010	1.852209	0.000000
O	0.932657	–2.026103	0.000000

H	3.162745	1.867183	0.000000
N	–2.760551	–1.510306	0.000000
C	–3.925300	–0.791832	0.000000
C	–2.791071	–2.878543	0.000000
N	–3.830738	0.560918	0.000000
C	–5.157977	–1.412028	0.000000
C	–5.258758	–2.868229	0.000000
C	–3.981994	–3.575568	0.000000
N	–1.604121	–3.534430	0.000000
H	–0.723586	–3.015305	0.000000
H	–2.916427	1.018167	0.000000
C	–4.929220	1.430837	0.000000
C	–1.471526	–4.929720	0.000000
H	–1.868740	–1.026501	0.000000
O	–0.353364	–5.424734	0.000000
C	–2.723460	–5.654489	0.000000
H	–2.661037	–6.734263	0.000000
C	–3.907170	–4.998930	0.000000
O	–4.735779	2.638614	0.000000
C	–6.218297	0.774796	0.000000
H	–7.090600	1.414269	0.000000
C	–6.311646	–0.575246	0.000000
H	–7.277859	–1.067225	0.000000
H	–4.845313	–5.542547	0.000000
O	–6.339683	–3.455516	0.000000
H	1.065332	2.933504	0.000000
H	3.257928	–0.637066	0.000000

Sum of electronic and thermal free energy: –1247.812547 a.u.
N_{Im}= 3 (93*i* cm^{-1}, 38*i* cm^{-1}, 12*i* cm^{-1})

13•8

	X	Y	Z
N	1.214429	1.990450	0.000000
C	0.004664	1.393751	0.000000
O	–0.015543	0.053652	0.000000
C	1.130720	–0.763039	0.000000
C	2.386637	–0.062155	0.000000
C	2.385712	1.279936	0.000000
N	–1.154879	1.971927	0.000000
O	0.932262	–1.943090	0.000000
H	3.289999	1.872589	0.000000
N	–2.866798	–1.538468	0.000000
C	–4.022754	–0.783173	0.000000
C	–2.857553	–2.919013	0.000000
N	–3.830211	0.544191	0.000000
C	–5.256419	–1.404242	0.000000
C	–5.382645	–2.911773	0.000000
C	–4.046523	–3.620983	0.000000
N	–1.637295	–3.477347	0.000000
H	–0.790492	–2.925144	0.000000

H	–2.903167	0.960209	0.000000
H	–4.665281	1.116317	0.000000
H	–1.603780	–4.488984	0.000000
H	–1.980721	–1.053070	0.000000
C	–6.435292	–0.598166	0.000000
C	–4.005501	–5.049115	0.000000
O	–7.580726	–1.324207	0.000000
O	–6.507131	0.634142	0.000000
H	–8.306451	–0.690111	0.000000
O	–5.235391	–5.620547	0.000000
O	–3.007451	–5.774693	0.000000
H	–5.094150	–6.573944	0.000000
H	–5.968059	–3.231221	0.869893
H	–5.968059	–3.231221	–0.869893
H	1.179815	3.012090	0.000000
H	3.296944	–0.640594	0.000000
C	–1.232263	3.347618	0.000000
H	–2.268281	3.707001	0.000000
O	–0.298515	4.133837	0.000000

Sum of electronic and thermal free energy: –1265.258891 a.u.
N_{Im}= 3 (37*i* cm^{-1}, 25*i* cm^{-1}, 19*i* cm^{-1})

14•8

	X	Y	Z
N	–2.212060	0.178985	0.000000
C	–1.053268	–0.645265	0.000000
N	0.141811	–0.024483	0.000000
C	0.205377	1.306933	0.000000
C	–0.952682	2.144538	0.000000
C	–2.179314	1.499382	0.000000
O	–1.225006	–1.856413	0.000000
N	1.450574	1.858381	0.000000
H	–3.125417	2.027234	0.000000
N	2.596329	–1.852604	0.000000
C	2.394451	–3.216317	0.000000
C	3.846790	–1.274416	0.000000
N	1.110532	–3.600565	0.000000
C	3.473918	–4.084376	0.000000
C	4.897412	–3.572595	0.000000
C	4.985671	–2.062678	0.000000
N	3.851108	0.066324	0.000000
H	2.995244	0.618167	0.000000
H	0.338529	–2.939355	0.000000
H	0.942478	–4.598417	0.000000
H	4.761903	0.507542	0.000000
H	1.779126	–1.237991	0.000000
C	3.234338	–5.489422	0.000000
C	6.264215	–1.433311	0.000000
O	4.374397	–6.229574	0.000000
O	2.146369	–6.074944	0.000000

H	4.097031	–7.152381	0.000000
O	7.298436	–2.314576	0.000000
O	6.515822	–0.223008	0.000000
H	8.104123	–1.786047	0.000000
H	5.431722	–3.972733	0.869847
H	5.431722	–3.972733	–0.869847
H	–3.096901	–0.313911	0.000000
C	–0.802563	3.553965	0.000000
H	–1.681091	4.189591	0.000000
C	0.457194	4.069741	0.000000
H	0.642206	5.135011	0.000000
C	1.549989	3.165306	0.000000
H	2.561756	3.562187	0.000000

Sum of electronic and thermal free energy: –1246.358048 a.u.
N_{Im}= 1 (18*i* cm^{-1})

ADD–DDA arrays

1•2

	X	Y	Z
C	0.020586	1.333619	0.000000
N	–0.005557	–0.001103	0.000000
C	1.145439	–0.712613	0.000000
O	1.181510	–1.945139	0.000000
N	2.344819	–0.008425	0.000000
C	2.394490	1.347564	0.000000
C	1.254831	2.068722	0.000000
N	–1.145042	1.977087	0.000000
C	–3.649202	–0.752394	0.000000
C	–4.826105	–1.555800	0.000000
C	–4.675038	–2.935501	0.000000
N	–3.539634	–3.658357	0.000000
C	–2.456709	–2.904696	0.000000
N	–2.492737	–1.533857	0.000000
O	–3.563329	0.477585	0.000000
N	–1.240561	–3.472445	0.000000
N	–6.163376	–1.206457	0.000000
C	–6.795680	–2.343898	0.000000
N	–5.947361	–3.427114	0.000000
H	3.380130	1.793744	0.000000
H	1.270339	3.148580	0.000000
H	–1.200118	–4.476484	0.000000
H	–0.375832	–2.926909	0.000000
H	–7.868113	–2.468963	0.000000
H	–2.026938	1.452700	0.000000
H	–1.169047	2.982067	0.000000
H	–1.599599	–1.011028	0.000000
H	3.190979	–0.557593	0.000000
H	–6.208186	–4.400251	0.000000

Sum of electronic and thermal free energy: –937.339217 a.u.

N_{Im}= 0

15•1

	X	Y	Z
C	0.040575	1.348411	0.000000
N	0.052208	–0.000233	0.000000
C	1.245817	–0.574444	0.000000
O	1.212477	–1.921494	0.000000
N	2.437603	–0.010508	0.000000
C	2.415011	1.337239	0.000000
C	1.260110	2.069372	0.000000
N	–1.147684	1.959823	0.000000
C	–3.657086	–0.774037	0.000000
C	–4.841465	–1.566443	0.000000
C	–4.707165	–2.946796	0.000000
N	–3.577576	–3.681084	0.000000
C	–2.489816	–2.940229	0.000000
N	–2.505754	–1.569532	0.000000
O	–3.559142	0.452198	0.000000
N	–1.280414	–3.529241	0.000000
N	–6.173661	–1.200684	0.000000
C	–6.819461	–2.330639	0.000000
N	–5.984153	–3.423904	0.000000
H	3.382286	1.829137	0.000000
H	1.271840	3.150628	0.000000
H	–1.249470	–4.533435	0.000000
H	–0.418225	–3.000060	0.000000
H	–7.893245	–2.442921	0.000000
H	–2.016920	1.419739	0.000000
H	–1.194427	2.963703	0.000000
H	–1.610974	–1.057794	0.000000
H	–6.256745	–4.393882	0.000000
H	2.122647	–2.238110	0.000000

Sum of electronic and thermal free energy: –937.322694 a.u.
N_{Im}= 0

2•16

	X	Y	Z
C	0.035615	1.388565	0.000000
N	–0.028266	0.056935	0.000000
C	1.106527	–0.687352	0.000000
O	1.108373	–1.916728	0.000000
N	2.323027	–0.010949	0.000000
C	2.407566	1.342088	0.000000
C	1.286254	2.092492	0.000000
N	–1.113205	2.066981	0.000000
C	–3.591050	–0.726603	0.000000
C	–4.823868	–1.544338	0.000000
C	–4.697793	–3.016658	0.000000
N	–3.614908	–3.676280	0.000000

C	–2.417782	–2.920640	0.000000
N	–2.476701	–1.507067	0.000000
O	–3.572574	0.491430	0.000000
N	–1.333368	–3.569574	0.000000
N	–6.054162	–1.199390	0.000000
C	–6.731105	–2.472054	0.000000
N	–6.004574	–3.531732	0.000000
H	3.403715	1.763915	0.000000
H	1.328894	3.171461	0.000000
H	–0.504347	–2.959250	0.000000
H	–7.813335	–2.485379	0.000000
H	–2.000517	1.567118	0.000000
H	–1.114290	3.072075	0.000000
H	–1.572153	–0.992637	0.000000
H	3.154875	–0.581799	0.000000

Sum of electronic and thermal free energy: –936.047107 a.u.
N_{Im}= 0

2•17

	X	Y	Z
C	0.030788	1.372456	0.000000
N	–0.041945	0.038656	0.000000
C	1.086394	–0.709332	0.000000
O	1.077592	–1.943963	0.000000
N	2.305937	–0.050146	0.000000
C	2.402118	1.303032	0.000000
C	1.287645	2.063117	0.000000
N	–1.111154	2.058831	0.000000
C	–3.624227	–0.717670	0.000000
C	–4.853424	–1.553341	0.000000
C	–4.719974	–3.052056	0.000000
N	–3.541803	–3.664250	0.000000
C	–2.469777	–2.871501	0.000000
N	–2.487442	–1.483852	0.000000
O	–3.605130	0.493940	0.000000
N	–1.273448	–3.421940	0.000000
N	–6.063084	–1.189861	0.000000
C	–6.786786	–2.504306	0.000000
N	–5.908887	–3.586109	0.000000
H	3.402267	1.715013	0.000000
H	1.341370	3.141681	0.000000
H	–1.235517	–4.429198	0.000000
H	–0.399347	–2.872517	0.000000
O	–7.982563	–2.536034	0.000000
H	–2.003988	1.571215	0.000000
H	–1.104823	3.064062	0.000000
H	–1.583788	–0.961846	0.000000
H	3.132857	–0.628622	0.000000

Sum of electronic and thermal free energy: –1011.332809 a.u.
N_{Im}= 0

18•1

	X	Y	Z
O	0.090953	–1.799855	0.000000
C	1.244475	–1.345009	0.000000
N	1.442828	0.028518	0.000000
C	2.656241	0.662879	0.000000
N	3.806391	0.018776	0.000000
C	3.650288	–1.318192	0.000000
C	2.473092	–2.058277	0.000000
N	2.742506	–3.413549	0.000000
C	4.041482	–3.484836	0.000000
N	4.646345	–2.248739	0.000000
N	2.622754	2.005716	0.000000
O	–2.219055	–0.578918	0.000000
C	–2.213316	0.726622	0.000000
N	–1.063861	1.374460	0.000000
C	–1.027598	2.735178	0.000000
N	–2.247488	3.397721	0.000000
C	–3.436873	2.745225	0.000000
C	–3.474067	1.393944	0.000000
O	0.019398	3.378054	0.000000
H	–2.214565	4.406688	0.000000
H	–4.323762	3.364634	0.000000
H	–1.292907	–0.970585	0.000000
H	0.573758	0.590721	0.000000
H	1.745748	2.525026	0.000000
H	3.499249	2.496939	0.000000
H	5.635913	–2.059155	0.000000
H	4.622231	–4.395000	0.000000
H	–4.399226	0.839274	0.000000

Sum of electronic and thermal free energy: –957.218095 a.u.
N_{Im}= 0

19•20

	X	Y	Z
C	–1.752875	1.676786	0.000000
C	–0.384235	1.275482	0.000000
N	–0.000952	0.013633	0.000000
C	–0.949463	–0.954696	0.000000
C	–2.332616	–0.657731	0.000000
C	–2.707658	0.708480	0.000000
N	0.651733	2.196104	0.000000
N	–0.497546	–2.233698	0.000000
C	–3.250093	–1.727101	0.000000
H	–3.759326	0.973805	0.000000
H	–1.997490	2.727296	0.000000
N	2.931720	–0.811833	0.000000
C	3.784492	0.280655	0.000000
C	3.324295	–2.116567	0.000000

O	3.286222	1.427078	0.000000
C	5.183369	–0.000169	0.000000
C	5.577868	–1.318359	0.000000
C	4.680313	–2.393718	0.000000
N	2.344838	–3.046688	0.000000
H	1.612512	1.804282	0.000000
C	0.586468	3.558582	0.000000
H	1.597542	3.993398	0.000000
O	–0.413206	4.248570	0.000000
H	–4.314733	–1.518798	0.000000
C	–2.776014	–3.012150	0.000000
H	–3.440944	–3.865814	0.000000
C	–1.382224	–3.207530	0.000000
H	1.927941	–0.588390	0.000000
C	6.142052	1.154338	0.000000
H	6.641511	–1.540532	0.000000
H	5.022061	–3.419395	0.000000
H	7.174015	0.796724	0.000000
H	5.999476	1.790783	0.878568
H	5.999476	1.790783	–0.878568
H	1.357620	–2.780228	0.000000
H	–0.981879	–4.217940	0.000000
H	2.597151	–4.018233	0.000000

Sum of electronic and thermal free energy: –1004.609319 a.u.
N_{Im}= 1 (64*i* cm^{-1})

19•21

	X	Y	Z
N	1.485651	–3.382498	0.000000
C	0.399834	–4.127452	0.000000
C	–0.910498	–3.617617	0.000000
C	–1.076210	–2.257894	0.000000
C	0.061932	–1.428239	0.000000
C	1.340144	–2.033451	0.000000
N	2.486027	–1.309664	0.000000
C	2.400728	0.007308	0.000000
C	1.160345	0.710913	0.000000
C	0.009337	–0.012483	0.000000
N	3.617586	0.668436	0.000000
C	3.864178	2.011409	0.000000
O	3.046990	2.908961	0.000000
O	4.653091	–7.030892	0.000000
C	3.802899	–6.165735	0.000000
N	4.005469	–4.819132	0.000000
C	5.230143	–4.163328	0.000000
C	6.466743	–4.747391	0.000000
C	7.596578	–3.899032	0.000000
C	7.510983	–2.535316	0.000000
C	6.205430	–1.934575	0.000000
N	5.132029	–2.800996	0.000000

O	5.999334	–0.706486	0.000000
C	8.700007	–1.623770	0.000000
H	–0.953865	0.485964	0.000000
H	1.163941	1.789498	0.000000
H	4.461174	0.068164	0.000000
H	4.947486	2.205302	0.000000
H	–2.064274	–1.810374	0.000000
H	–1.753206	–4.296082	0.000000
H	4.205581	–2.349883	0.000000
H	8.578846	–4.361798	0.000000
H	6.560032	–5.819837	0.000000
H	9.627620	–2.198669	0.000000
H	8.693199	–0.971944	0.878100
H	8.693199	–0.971944	–0.878100
H	3.147856	–4.241737	0.000000
H	2.727304	–6.402794	0.000000
H	0.553457	–5.202853	0.000000

Sum of electronic and thermal free energy: –1117.932594 a.u.
N_{Im}= 1 (15*i* cm^{-1})

19•22

	X	Y	Z
N	0.649986	–2.189747	0.000000
C	0.345468	–3.469962	0.000000
C	–0.969431	–3.971143	0.000000
C	–2.004571	–3.074226	0.000000
C	–1.717020	–1.694883	0.000000
C	–0.362648	–1.287459	0.000000
N	0.001039	0.018807	0.000000
C	–0.944542	0.937994	0.000000
C	–2.336502	0.629229	0.000000
C	–2.705077	–0.679741	0.000000
N	–0.483709	2.245611	0.000000
C	–1.198831	3.409170	0.000000
O	–2.406696	3.527536	0.000000
N	3.514522	–1.554434	0.000000
C	3.939420	–0.281655	0.000000
N	5.228372	–0.009165	0.000000
C	5.481778	1.313825	0.000000
C	4.580441	2.369581	0.000000
C	3.191227	2.063865	0.000000
O	2.235930	2.844088	0.000000
N	2.964214	0.685312	0.000000
N	5.244910	3.578937	0.000000
C	6.505286	3.249540	0.000000
N	6.717481	1.889492	0.000000
H	–3.753986	–0.955283	0.000000
H	–3.057867	1.431079	0.000000
H	4.213588	–2.276149	0.000000
H	2.517847	–1.789797	0.000000

C	7.988169	1.190618	0.000000
H	7.336366	3.940432	0.000000
H	0.541034	2.364519	0.000000
H	–3.037671	–3.405164	0.000000
H	–1.140004	–5.039634	0.000000
H	1.975697	0.398729	0.000000
H	–0.523820	4.278181	0.000000
H	8.790653	1.926837	0.000000
H	1.183951	–4.161283	0.000000
H	8.073108	0.564766	0.889039
H	8.073108	0.564766	–0.889039

Sum of electronic and thermal free energy: –1168.271484 a.u.
N_{Im}= 0

23•24

	X	Y	Z
O	3.544730	2.011149	0.000000
C	2.431258	1.326108	0.000000
C	1.209789	2.078147	0.000000
C	0.030469	1.413799	0.000000
C	0.024064	–0.011316	0.000000
C	1.275381	–0.670472	0.000000
N	2.453842	0.007147	0.000000
C	–1.143846	–0.790007	0.000000
C	–1.038371	–2.159994	0.000000
C	0.244556	–2.724112	0.000000
N	1.363623	–2.022362	0.000000
N	5.793731	0.725767	0.000000
C	6.043539	–0.550076	0.000000
C	7.356469	–1.176550	0.000000
C	7.430742	–2.530830	0.000000
C	6.278934	–3.372361	0.000000
C	5.045635	–2.746476	0.000000
N	4.957353	–1.393436	0.000000
C	6.367667	–4.827547	0.000000
O	7.448069	–5.429749	0.000000
C	5.082252	–5.506856	0.000000
C	3.921868	–4.812577	0.000000
N	3.885368	–3.449271	0.000000
H	–0.912576	1.949526	0.000000
H	1.269944	3.158314	0.000000
H	2.980045	–2.945564	0.000000
H	–2.112584	–0.301386	0.000000
H	–1.911060	–2.799461	0.000000
C	8.567509	–0.292098	0.000000
H	8.397731	–3.023212	0.000000
H	8.589120	0.355094	–0.883282
H	8.589120	0.355094	0.883282
H	9.478289	–0.891405	0.000000
H	6.637713	1.284294	0.000000

H	2.954241	–5.297471	0.000000
H	5.067443	–6.588761	0.000000
H	0.356913	–3.804381	0.000000
H	4.411272	1.429571	0.000000
H	4.025278	–0.936669	0.000000

Sum of electronic and thermal free energy: –1080.794783 a.u.
N_{Im}= 0

25•26

	X	Y	Z
C	1.223246	2.110131	0.000000
C	0.028444	1.351621	0.000000
N	–0.003570	–0.011056	0.000000
C	1.167357	–0.633176	0.000000
C	2.445545	–0.013924	0.000000
C	2.526816	1.448019	0.000000
N	–1.178579	1.963008	0.000000
N	1.142171	–2.003578	0.000000
C	3.583906	–0.807183	0.000000
O	3.595726	2.055404	0.000000
N	–2.516036	–1.432623	0.000000
C	–3.711770	–0.801752	0.000000
C	–2.435291	–2.816427	0.000000
N	–3.712763	0.526430	0.000000
N	–4.858966	–1.480913	0.000000
C	–4.713891	–2.813504	0.000000
N	–3.610116	–3.522110	0.000000
N	–1.258781	–3.348428	0.000000
H	–2.831638	1.061536	0.000000
H	–5.643767	–3.378039	0.000000
H	–4.605247	0.990387	0.000000
H	–1.343152	–4.359557	0.000000
C	1.128068	3.503972	0.000000
C	–1.249257	3.288859	0.000000
C	–2.628334	3.886231	0.000000
C	–0.108096	4.106250	0.000000
C	2.237088	–2.776622	0.000000
C	2.017623	–4.256185	0.000000
C	3.494211	–2.191230	0.000000
H	–2.592692	4.975594	0.000000
H	–3.181675	3.556597	–0.883312
H	–3.181675	3.556597	0.883312
H	2.969981	–4.783462	0.000000
H	1.446057	–4.554767	0.881862
H	1.446057	–4.554767	–0.881862
H	4.548796	–0.311818	0.000000
H	4.376261	–2.816218	0.000000
H	2.043592	4.084921	0.000000
H	–0.211989	5.183692	0.000000
H	–1.628371	–0.889283	0.000000

H	0.192091	–2.489019	0.000000

Sum of electronic and thermal free energy: –1132.331766 a.u.
N_{Im}= 0

ADA–DAD arrays

27•28

	X	Y	Z
O	6.100060	0.388325	0.000000
C	6.108294	–0.836594	0.000000
C	7.306382	–1.650528	0.000000
C	7.191917	–2.989608	0.000000
N	5.968367	–3.601193	0.000000
C	4.779830	–2.907627	0.000000
N	4.912296	–1.543691	0.000000
O	3.700693	–3.477435	0.000000
N	3.668076	1.957756	0.000000
C	2.475360	1.349231	0.000000
N	2.411837	0.008362	0.000000
C	1.192413	–0.592292	0.000000
N	–0.004242	0.006610	0.000000
C	0.101490	1.336567	0.000000
C	1.270289	2.080064	0.000000
N	1.194704	–1.944207	0.000000
N	1.001729	3.438134	0.000000
C	–0.299182	3.504277	0.000000
N	–0.901899	2.267305	0.000000
H	8.045322	–3.654517	0.000000
H	8.267777	–1.160565	0.000000
H	4.026707	–0.995784	0.000000
H	0.310371	–2.419656	0.000000
H	2.056914	–2.476544	0.000000
H	3.699330	2.962772	0.000000
H	4.535724	1.425320	0.000000
H	–0.882298	4.413091	0.000000
H	5.894413	–4.606989	0.000000
H	–1.891565	2.080066	0.000000

Sum of electronic and thermal free energy: –937.341038 a.u.
N_{Im}= 1 (46*i* cm^{-1})

27•29

	X	Y	Z
O	–3.724890	0.220101	0.000000
C	–3.502179	1.422926	0.000000
C	–4.513348	2.460245	0.000000
C	–4.133319	3.749266	0.000000
N	–2.810614	4.107474	0.000000
C	–1.791920	3.190381	0.000000
N	–2.190341	1.885419	0.000000
O	–0.612928	3.529078	0.000000

N	–1.542612	–1.747628	0.000000
C	–0.269627	–1.346825	0.000000
N	–0.002168	–0.026235	0.000000
C	1.283314	0.361259	0.000000
C	2.426183	–0.495250	0.000000
C	2.118085	–1.892155	0.000000
C	0.783193	–2.298028	0.000000
N	1.514648	1.701419	0.000000
H	–4.836667	4.571107	0.000000
H	–5.553789	2.174111	0.000000
H	–1.427594	1.177801	0.000000
H	0.697042	2.332292	0.000000
H	–1.727074	–2.737403	0.000000
H	–2.317458	–1.087941	0.000000
C	3.693124	0.069357	0.000000
C	2.740339	2.249685	0.000000
H	2.773413	3.330407	0.000000
C	3.860215	1.453410	0.000000
H	4.841946	1.905198	0.000000
H	4.553889	–0.589514	0.000000
N	0.722720	–3.659299	0.000000
H	–2.539635	5.079149	0.000000
N	2.915140	–2.981126	0.000000
C	2.017928	–3.993063	0.000000
H	2.338475	–5.028028	0.000000

Sum of electronic and thermal free energy: –1035.550255 a.u.
N_{Im}= 0

30•31

	X	Y	Z
C	7.284853	–1.664920	0.000000
C	6.096358	–0.828168	0.000000
N	4.913689	–1.545496	0.000000
C	4.776070	–2.910788	0.000000
N	5.953679	–3.632457	0.000000
C	7.167680	–3.006101	0.000000
O	6.097851	0.392140	0.000000
O	3.689207	–3.464839	0.000000
C	2.477154	1.355687	0.000000
C	1.273001	2.086446	0.000000
C	0.104265	1.343213	0.000000
N	–0.001895	0.012497	0.000000
C	1.194164	–0.586499	0.000000
N	2.414931	0.013552	0.000000
N	3.668950	1.966716	0.000000
N	1.194383	–1.938702	0.000000
N	1.000290	3.441865	0.000000
C	–0.302832	3.497621	0.000000
N	–0.909050	2.262319	0.000000
C	5.847415	–5.091543	0.000000

H	8.035985	–3.651816	0.000000
Cl	8.834569	–0.897024	0.000000
H	4.025544	–0.997602	0.000000
H	6.850607	–5.511867	0.000000
H	5.311071	–5.424944	0.887810
H	5.311071	–5.424944	–0.887810
H	0.308632	–2.411484	0.000000
H	2.055332	–2.472387	0.000000
H	3.697885	2.971812	0.000000
H	4.537197	1.437808	0.000000
C	–2.329005	1.972360	0.000000
H	–0.892192	4.403641	0.000000
H	–2.878447	2.912844	0.000000
H	–2.596043	1.399053	–0.888675
H	–2.596043	1.399053	0.888675

Sum of electronic and thermal free energy: –1475.514352 a.u.
N_{Im}= 1 (48*i* cm^{-1})

32•33

	X	Y	Z
C	1.237822	–0.769496	0.000000
O	1.316128	–1.993666	0.000000
N	2.392389	–0.002460	0.000000
C	2.466655	1.365025	0.000000
O	3.534800	1.961554	0.000000
N	1.260632	2.030580	0.000000
C	0.078236	1.339346	0.000000
C	0.014784	–0.005589	0.000000
N	5.015137	–1.462517	0.000000
C	5.058841	–2.806378	0.000000
C	6.236500	–3.534334	0.000000
C	7.435726	–2.821624	0.000000
C	7.424324	–1.430037	0.000000
C	6.179221	–0.806867	0.000000
O	8.555549	–3.556691	0.000000
N	6.052148	0.584989	0.000000
C	7.030334	1.531004	0.000000
O	8.231430	1.346297	0.000000
N	3.800560	–3.412841	0.000000
C	3.497450	–4.739492	0.000000
O	4.277842	–5.670521	0.000000
C	1.299639	3.492412	0.000000
H	–0.813840	1.952382	0.000000
H	–0.930803	–0.525450	0.000000
H	3.296946	–0.503440	0.000000
H	0.277630	3.864645	0.000000
H	1.819085	3.851860	0.887791
H	1.819085	3.851860	–0.887791
H	5.101421	0.959181	0.000000
H	2.986662	–2.792883	0.000000

C	9.811233	–2.887904	0.000000
H	10.563096	–3.673560	0.000000
H	9.925787	–2.270159	–0.894782
H	9.925787	–2.270159	0.894782
H	2.406413	–4.889514	0.000000
H	6.594281	2.542154	0.000000
H	6.230959	–4.612325	0.000000
H	8.318082	–0.829736	0.000000

Sum of electronic and thermal free energy: –1154.103285 a.u.
N_{Im}= 0

34•35

	X	Y	Z
O	1.323462	–1.986778	0.000000
C	1.252308	–0.761134	0.000000
N	2.408792	–0.003283	0.000000
C	2.493067	1.364270	0.000000
O	3.567975	1.951985	0.000000
N	1.292962	2.027554	0.000000
C	0.103054	1.338671	0.000000
C	0.013746	–0.006243	0.000000
O	4.244751	–5.688787	0.000000
C	3.474796	–4.749173	0.000000
N	3.791970	–3.425331	0.000000
C	5.056752	–2.833100	0.000000
N	5.036279	–1.494460	0.000000
C	6.201680	–0.836010	0.000000
C	7.437636	–1.481267	0.000000
C	7.430406	–2.866392	0.000000
C	6.239100	–3.572731	0.000000
N	6.073190	0.555207	0.000000
C	7.054184	1.499006	0.000000
O	8.254077	1.310514	0.000000
C	1.329081	3.488812	0.000000
H	–0.781565	1.963620	0.000000
C	–1.285825	–0.749904	0.000000
H	3.307311	–0.510826	0.000000
H	0.305974	3.858060	0.000000
H	1.847352	3.850606	0.887731
H	1.847352	3.850606	–0.887731
H	5.123605	0.933243	0.000000
H	2.983166	–2.797950	0.000000
H	2.382216	–4.887061	0.000000
H	6.207351	–4.650255	0.000000
H	8.351174	–0.908956	0.000000
H	6.620121	2.511167	0.000000
H	–2.129221	–0.057843	0.000000
H	–1.363631	–1.393457	–0.879696
H	–1.363631	–1.393457	0.879696
H	8.370854	–3.405381	0.000000

Sum of electronic and thermal free energy: –1078.895486 a.u.
N_{Im}= 1 (19*i* cm^{-1})

27•36

	X	Y	Z
O	2.757872	2.990626	0.000000
C	1.942573	2.083489	0.000000
N	2.295908	0.760334	0.000000
C	1.436653	–0.321823	0.000000
O	1.895415	–1.463280	0.000000
N	0.584780	2.307777	0.000000
C	–0.338581	1.298659	0.000000
C	0.029214	0.004172	0.000000
N	5.072863	0.015163	0.000000
C	6.057323	0.955567	0.000000
N	7.371835	0.724012	0.000000
C	7.658288	–0.576510	0.000000
C	6.756270	–1.638052	0.000000
C	5.403312	–1.274599	0.000000
O	4.470933	–2.202668	0.000000
N	5.655033	2.245147	0.000000
N	8.890251	–1.166051	0.000000
C	8.679346	–2.526751	0.000000
N	7.420680	–2.853592	0.000000
H	0.292654	3.273194	0.000000
H	–1.373349	1.614318	0.000000
H	4.675689	2.505334	0.000000
H	6.359278	2.961225	0.000000
H	9.779521	–0.692854	0.000000
H	9.506783	–3.220793	0.000000
H	3.314330	0.543564	0.000000
H	3.555308	–1.828966	0.000000
H	–0.695664	–0.794933	0.000000

Sum of electronic and thermal free energy: –957.217847 a.u.
N_{Im}= 1 (33*i* cm^{-1})

37•38

	X	Y	Z
C	–4.289548	0.767661	0.000000
C	–3.133062	–0.119129	0.000000
N	–1.904116	0.495978	0.000000
C	–1.719018	1.854473	0.000000
C	–2.838521	2.706012	0.000000
C	–4.145024	2.105942	0.000000
O	–3.222645	–1.347205	0.000000
N	–0.458240	2.298622	0.000000
C	–2.601782	4.081941	0.000000
H	–5.013384	2.756391	0.000000
H	–5.260473	0.290386	0.000000
N	0.482934	–1.324730	0.000000

C	0.314643	–2.650514	0.000000
C	1.738876	–0.846551	0.000000
N	–0.950959	–3.113474	0.000000
C	1.412720	–3.574666	0.000000
C	2.669771	–3.043125	0.000000
C	2.881800	–1.650031	0.000000
N	1.876784	0.515909	0.000000
C	3.104345	1.093578	0.000000
H	1.034304	1.103825	0.000000
H	–3.441679	4.768022	0.000000
C	–1.301283	4.547779	0.000000
H	–1.078072	5.606149	0.000000
C	–0.267075	3.614079	0.000000
C	1.158104	–5.054752	0.000000
H	3.542965	–3.686917	0.000000
C	4.226552	–1.071710	0.000000
H	2.100518	–5.603212	0.000000
H	–1.131177	–4.100717	0.000000
H	–1.745741	–2.474982	0.000000
H	–1.068402	–0.114495	0.000000
H	3.102843	2.176714	0.000000
C	4.254417	0.376388	0.000000
O	5.248398	–1.770454	0.000000
H	5.210793	0.882093	0.000000
H	0.766819	3.944044	0.000000
H	0.591747	–5.366451	0.884449
H	0.591747	–5.366451	–0.884449

Sum of electronic and thermal free energy: –1080.813975 a.u.
N_{Im}= 1 (10*i* cm^{-1})

39•40

	X	Y	Z
N	–1.085257	–0.790565	0.000000
C	–2.264589	–0.186690	0.000000
C	–2.429209	1.202224	0.000000
C	–1.303828	1.995442	0.000000
C	–0.039988	1.389558	0.000000
C	0.003715	–0.013672	0.000000
N	1.216527	–0.647156	0.000000
C	2.414425	–0.009699	0.000000
C	2.384765	1.431959	0.000000
C	1.203424	2.092227	0.000000
N	3.473743	–0.810149	0.000000
C	4.761685	–0.342653	0.000000
O	5.163979	0.808564	0.000000
O	–2.578101	–5.408073	0.000000
C	–2.237642	–4.240872	0.000000
N	–0.972802	–3.750643	0.000000
C	0.236438	–4.457249	0.000000
C	0.309020	–5.840263	0.000000

C	1.579593	–6.414614	0.000000
C	2.721162	–5.640892	0.000000
C	2.525243	–4.245001	0.000000
N	1.325682	–3.666609	0.000000
O	3.613386	–3.485031	0.000000
H	1.189869	3.176885	0.000000
H	3.330077	1.949402	0.000000
H	5.479917	–1.178553	0.000000
H	–1.379280	3.077001	0.000000
H	–3.423337	1.628362	0.000000
C	4.108588	–6.212193	0.000000
H	1.670005	–7.496304	0.000000
H	–0.588533	–6.437034	0.000000
H	4.073701	–7.303092	0.000000
H	4.670435	–5.883730	0.878639
H	4.670435	–5.883730	–0.878639
H	–0.904466	–2.728993	0.000000
H	–2.976127	–3.422323	0.000000
H	–3.133843	–0.836639	0.000000
H	1.225721	–1.683355	0.000000
H	3.416387	–2.502700	0.000000

Sum of electronic and thermal free energy: –1117.918581 a.u.
N_{Im}= 1 (3*i* cm^{-1})

41•42

	X	Y	Z
C	–2.390812	–1.469490	0.000000
C	–1.137269	–2.105204	0.000000
N	0.017546	–1.372392	0.000000
C	0.003970	–0.004757	0.000000
C	–1.211502	0.701024	0.000000
C	–2.497816	–0.005716	0.000000
N	–0.998564	–3.436898	0.000000
N	1.196721	0.603515	0.000000
C	–1.143183	2.095168	0.000000
O	–3.574596	0.579333	0.000000
H	0.924238	–1.865027	0.000000
N	2.666230	–2.811507	0.000000
C	2.758213	–4.150607	0.000000
C	3.839770	–2.160007	0.000000
N	1.620715	–4.854263	0.000000
N	3.918736	–4.842934	0.000000
C	5.000518	–4.079800	0.000000
N	5.052124	–2.756939	0.000000
N	3.811156	–0.822765	0.000000
H	2.921426	–0.322124	0.000000
H	0.716535	–4.380216	0.000000
H	5.956247	–4.599078	0.000000
H	1.680496	–5.857548	0.000000
H	4.685429	–0.326981	0.000000

C	–3.523304	–2.285435	0.000000
C	–2.090091	–4.198999	0.000000
C	–1.865956	–5.682959	0.000000
C	–3.382075	–3.655372	0.000000
C	1.242157	1.933990	0.000000
C	2.609144	2.553443	0.000000
C	0.083026	2.722132	0.000000
H	–2.808391	–6.230126	0.000000
H	–1.291304	–5.975174	–0.882700
H	–1.291304	–5.975174	0.882700
H	2.555382	3.641876	0.000000
H	3.167006	2.230327	0.882700
H	3.167006	2.230327	–0.882700
H	–2.069553	2.658027	0.000000
H	0.162323	3.801466	0.000000
H	–4.499622	–1.814503	0.000000
H	–4.244473	–4.309223	0.000000

Sum of electronic and thermal free energy: –1132.353147 a.u.
N_{Im}= 1 (15*i* cm^{-1})

Monomers

1

	X	Y	Z
C	0.017634	1.313342	0.000000
N	–0.014515	–0.008091	0.000000
C	1.145825	–0.718691	0.000000
O	1.205955	–1.940839	0.000000
N	2.344027	0.012468	0.000000
C	2.383452	1.365243	0.000000
C	1.234536	2.075017	0.000000
N	–1.161950	1.960930	0.000000
H	3.364380	1.822385	0.000000
H	1.235539	3.155110	0.000000
H	–2.013067	1.424237	0.000000
H	–1.214247	2.963793	0.000000
H	3.195742	–0.527882	0.000000

Sum of electronic and thermal free energy: –394.863293 a.u.
N_{Im}= 0

2

	X	Y	Z
C	0.212090	–1.399931	0.000000
C	–1.041894	–2.088016	0.000000
C	–2.208767	–1.340168	0.000000
N	–2.354520	0.003334	0.000000
C	–1.208140	0.638509	0.000000
N	0.004382	–0.000644	0.000000

O	1.348364	–1.840066	0.000000
N	–1.191766	1.988153	0.000000
N	–1.324177	–3.439122	0.000000
C	–2.624752	–3.499662	0.000000
N	–3.215586	–2.258153	0.000000
H	–2.072204	2.472473	0.000000
H	–0.342056	2.522832	0.000000
H	–3.213682	–4.404415	0.000000
H	0.855330	0.544975	0.000000
H	–4.202971	–2.057199	0.000000

Sum of electronic and thermal free energy: –542.462866 a.u.
N_{Im}= 1 (229*i* cm^{-1})

7

	X	Y	Z
C	–1.094231	–2.189104	0.000000
C	–1.147905	–0.757685	0.000000
N	–2.294356	–0.078753	0.000000
C	–3.440807	–0.757685	0.000000
C	–3.494481	–2.189104	0.000000
C	–2.294356	–2.890140	0.000000
N	–0.002125	–0.002826	0.000000
N	–4.586587	–0.002826	0.000000
C	–4.771572	–2.820739	0.000000
H	–2.294356	–3.976113	0.000000
C	0.182860	–2.820739	0.000000
C	1.140512	–0.628686	0.000000
C	1.297325	–2.046044	0.000000
C	–5.729224	–0.628686	0.000000
C	–5.886036	–2.046044	0.000000
H	–4.829406	–3.903892	0.000000
H	–6.880406	–2.473835	0.000000
H	0.240695	–3.903892	0.000000
H	2.291694	–2.473835	0.000000
H	–6.619690	–0.004246	0.000000
H	2.030979	–0.004247	0.000000

Sum of electronic and thermal free energy: –587.452080 a.u.
N_{Im}= 0

8

	X	Y	Z
N	1.261290	2.045936	0.000000
C	0.045316	1.392233	0.000000
C	2.477715	1.393073	0.000000
N	–1.031951	2.198608	0.000000
C	–0.000783	0.016626	0.000000
C	1.262278	–0.816054	0.000000
C	2.524763	0.017498	0.000000
N	3.554425	2.200191	0.000000
C	–1.277561	–0.632206	0.000000

C	3.801989	–0.630452	0.000000
O	–1.189072	–1.982260	0.000000
O	–2.388029	–0.097870	0.000000
H	–2.092003	–2.319939	0.000000
O	3.714434	–1.980567	0.000000
O	4.912088	–0.095348	0.000000
H	4.617597	–2.317622	0.000000
H	1.260942	3.053016	0.000000
H	4.463042	1.753212	0.000000
H	3.470233	3.200874	0.000000
H	–1.940259	1.751002	0.000000
H	–0.948449	3.199348	0.000000
H	1.262508	–1.481610	0.870420
H	1.262508	–1.481610	–0.870420

Sum of electronic and thermal free energy: –737.228532 a.u.
N_{Im}= 3 (276*i* cm^{-1}, 218*i* cm^{-1}, 15*i* cm^{-1})

9

	X	Y	Z
C	4.134073	5.019739	0.000000
C	2.916137	4.285921	0.000000
N	2.877265	2.956554	0.000000
C	4.017407	2.271863	0.000000
C	5.292473	2.901198	0.000000
C	5.316479	4.290297	0.000000
N	1.677064	4.906632	0.000000
N	3.871282	0.893737	0.000000
C	6.483331	2.068459	0.000000
H	6.266009	4.809492	0.000000
C	4.075676	6.471698	0.000000
C	1.645837	6.195564	0.000000
C	2.799078	7.059772	0.000000
C	4.939553	0.171852	0.000000
C	6.289478	0.676354	0.000000
C	7.799181	2.563152	0.000000
C	7.389207	–0.198284	0.000000
C	5.202270	7.312513	0.000000
C	2.656229	8.457624	0.000000
H	4.803104	–0.909119	0.000000
H	0.662154	6.664057	0.000000
H	7.215023	–1.269106	0.000000
C	8.670286	0.305333	0.000000
C	8.869802	1.693835	0.000000
H	7.988445	3.629378	0.000000
H	9.878883	2.089751	0.000000
H	9.522286	–0.363896	0.000000
C	5.048191	8.682988	0.000000
H	1.660725	8.888871	0.000000
C	3.771570	9.264351	0.000000
H	6.202041	6.896442	0.000000

H	5.926073	9.318847	0.000000
H	3.667958	10.342792	0.000000

Sum of electronic and thermal free energy: –894.625341 a.u.
N_{Im}= 0

10

	X	Y	Z
O	1.235363	2.023808	0.000000
C	0.037574	1.390764	0.000000
C	2.492258	1.399276	0.000000
O	–0.985748	2.014187	0.000000
N	0.102000	0.017789	0.000000
C	1.280216	–0.676890	0.000000
C	2.463603	–0.044299	0.000000
O	3.448741	2.117549	0.000000
H	–0.782522	–0.466932	0.000000
H	3.400865	–0.577830	0.000000
H	1.187739	–1.754572	0.000000

Sum of electronic and thermal free energy: –434.619632 a.u.
N_{Im}= 0

11

	X	Y	Z
N	1.261290	2.045558	0.000000
C	0.059040	1.378172	0.000000
C	2.464001	1.379003	0.000000
N	–1.050249	2.169605	0.000000
C	0.038008	0.014298	0.000000
C	1.262257	–0.753865	0.000000
C	2.485976	0.015144	0.000000
N	3.572743	2.171202	0.000000
H	1.260942	3.052831	0.000000
H	4.482877	1.748840	0.000000
H	3.520126	3.173668	0.000000
H	–1.960091	1.746613	0.000000
H	–0.998324	3.172107	0.000000
O	1.262688	–2.000247	0.000000
H	–0.909814	–0.508620	0.000000
H	3.434159	–0.507119	0.000000

Sum of electronic and thermal free energy: –434.131744 a.u.
N_{Im}= 2 (443*i* cm^{-1}, 425*i* cm^{-1})

12

	X	Y	Z
C	3.876325	–1.424240	0.000000
C	2.769496	–2.243427	0.000000
N	1.499847	–1.735125	0.000000
C	1.293324	–0.383190	0.000000
C	2.342574	0.508557	0.000000
C	3.724294	0.030062	0.000000

N	2.908002	–3.593287	0.000000
N	0.010242	0.058404	0.000000
C	2.019525	1.898001	0.000000
O	4.685976	0.793195	0.000000
C	5.156026	–2.054544	0.000000
C	4.138883	–4.269639	0.000000
C	5.294893	–3.400704	0.000000
C	–0.368744	1.410768	0.000000
C	0.740127	2.339106	0.000000
H	2.848249	2.597012	0.000000
H	0.492619	3.391814	0.000000
H	6.025052	–1.406322	0.000000
H	6.263829	–3.880931	0.000000
O	–1.556468	1.693103	0.000000
O	4.143963	–5.490448	0.000000
H	–0.761574	–0.597170	0.000000
H	0.710253	–2.361699	0.000000
H	2.094206	–4.195958	0.000000

Sum of electronic and thermal free energy: –813.195914 a.u.
N_{Im}= 1 (577*i* cm^{-1})

13

	X	Y	Z
O	1.169502	–0.644506	0.000000
C	0.000040	0.001879	0.000000
C	2.431284	–0.019806	0.000000
N	–1.063213	–0.741495	0.000000
N	0.041525	1.354464	0.000000
C	1.218350	2.055430	0.000000
C	2.401479	1.423897	0.000000
O	3.382594	–0.741185	0.000000
H	–0.878444	1.799845	0.000000
H	3.340013	1.955689	0.000000
H	1.119581	3.132266	0.000000
C	–2.299823	–0.149833	0.000000
H	–3.114029	–0.885211	0.000000
O	–2.555240	1.048967	0.000000

Sum of electronic and thermal free energy: –528.032229 a.u.
N_{Im}= 0

14

	X	Y	Z
N	–2.015164	1.107974	0.000000
C	–2.748514	–0.120693	0.000000
N	–2.023649	–1.259412	0.000000
C	–0.697195	–1.210854	0.000000
C	0.046499	0.016607	0.000000
C	–0.695169	1.184306	0.000000
O	–3.965572	–0.040547	0.000000
N	–0.036856	–2.411329	0.000000

H	–0.246554	2.171064	0.000000
H	–2.578412	1.948904	0.000000
C	1.465327	–0.012338	0.000000
H	2.023698	0.917684	0.000000
C	2.084301	–1.222039	0.000000
H	3.161669	–1.318193	0.000000
C	1.269603	–2.389614	0.000000
H	1.758248	–3.361460	0.000000

Sum of electronic and thermal free energy: –509.117608 a.u.
N_{Im}= 0

15

	X	Y	Z
C	0.048752	1.334464	0.000000
N	0.058009	–0.004172	0.000000
C	1.250643	–0.578857	0.000000
O	1.228587	–1.918724	0.000000
N	2.443527	0.002185	0.000000
C	2.413169	1.344805	0.000000
C	1.251303	2.074067	0.000000
N	–1.158003	1.936395	0.000000
H	3.377469	1.843464	0.000000
H	1.256090	3.155602	0.000000
H	–1.989469	1.370886	0.000000
H	–1.245106	2.936543	0.000000
H	2.144500	–2.217189	0.000000

Sum of electronic and thermal free energy: –394.855832 a.u.
N_{Im}= 0

16

	X	Y	Z
C	–3.601468	–0.705604	0.000000
C	–4.833756	–1.528152	0.000000
C	–4.709263	–3.005127	0.000000
N	–3.630376	–3.670802	0.000000
C	–2.430564	–2.925572	0.000000
N	–2.486147	–1.516171	0.000000
O	–3.550542	0.498901	0.000000
N	–1.351360	–3.588363	0.000000
N	–6.061478	–1.182879	0.000000
C	–6.741912	–2.457995	0.000000
N	–6.016275	–3.517051	0.000000
H	–0.527786	–2.988992	0.000000
H	–7.824051	–2.468689	0.000000
H	–1.601910	–1.023815	0.000000

Sum of electronic and thermal free energy: –541.174563 a.u.
N_{Im}= 0

17

	X	Y	Z

C	0.268635	–1.376595	0.000000
C	–1.019705	–2.119843	0.000000
C	–2.316164	–1.353569	0.000000
N	–2.363807	–0.019030	0.000000
C	–1.199767	0.606032	0.000000
N	0.043963	–0.004131	0.000000
O	1.371069	–1.851199	0.000000
N	–1.197496	1.933297	0.000000
N	–1.213452	–3.367700	0.000000
C	–2.708534	–3.454740	0.000000
N	–3.308372	–2.188816	0.000000
H	–2.088482	2.404092	0.000000
H	–0.356934	2.486862	0.000000
O	–3.258052	–4.514109	0.000000
H	0.877989	0.569319	0.000000

Sum of electronic and thermal free energy: –616.452206 a.u.
N_{Im}= 0

18

	X	Y	Z
C	0.015812	0.003473	0.000000
N	1.254378	–0.652187	0.000000
C	2.441748	–0.004870	0.000000
C	2.475574	1.348513	0.000000
C	1.205047	1.987723	0.000000
N	0.054091	1.373306	0.000000
O	–1.010540	–0.653107	0.000000
O	1.206375	3.318442	0.000000
H	1.221592	–1.661141	0.000000
H	3.329982	–0.622586	0.000000
H	0.287261	3.614913	0.000000
H	3.396289	1.910161	0.000000

Sum of electronic and thermal free energy: –414.739358 a.u.
N_{Im}= 0

19

	X	Y	Z
C	–0.008319	–0.018768	0.000000
C	0.779109	1.165007	0.000000
N	2.089162	1.181001	0.000000
C	2.751356	–0.001291	0.000000
C	2.065402	–1.241203	0.000000
C	0.650275	–1.211655	0.000000
N	0.202440	2.440776	0.000000
N	4.106178	0.073077	0.000000
C	2.827079	–2.429374	0.000000
H	0.096697	–2.144419	0.000000
H	–1.085180	0.047514	0.000000
H	0.884024	3.187434	0.000000
C	–1.112092	2.807657	0.000000

H	–1.218004	3.903432	0.000000
O	–2.068291	2.063180	0.000000
H	2.322637	–3.389923	0.000000
C	4.191719	–2.338874	0.000000
H	4.821209	–3.219521	0.000000
C	4.778782	–1.054565	0.000000
H	5.862177	–0.965764	0.000000

Sum of electronic and thermal free energy: –586.513324 a.u.
N_{Im}= 0

20

	X	Y	Z
N	2.949435	–0.812744	0.000000
C	3.789782	0.305616	0.000000
C	3.345751	–2.116990	0.000000
O	3.276980	1.427390	0.000000
C	5.197193	0.011766	0.000000
C	5.591394	–1.300655	0.000000
C	4.695122	–2.387446	0.000000
N	2.368162	–3.060779	0.000000
H	1.963526	–0.588231	0.000000
C	6.152462	1.168098	0.000000
H	6.655154	–1.521598	0.000000
H	5.044759	–3.410251	0.000000
H	7.185792	0.815046	0.000000
H	6.005209	1.803744	0.878261
H	6.005209	1.803744	–0.878261
H	1.393052	–2.821302	0.000000
H	2.613929	–4.033778	0.000000

Sum of electronic and thermal free energy: –418.084793 a.u.
N_{Im}= 1 (370*i* cm^{-1})

21

	X	Y	Z
N	2.306104	1.395870	0.000000
C	2.423490	0.007792	0.000000
C	1.132746	2.098705	0.000000
O	3.543829	–0.498595	0.000000
C	1.167149	–0.710406	0.000000
C	0.005295	0.001722	0.000000
C	–0.048264	1.420213	0.000000
N	1.291210	3.485126	0.000000
H	3.194237	1.880538	0.000000
C	1.228568	–2.207028	0.000000
H	–0.937526	–0.536573	0.000000
H	–0.983912	1.952558	0.000000
H	0.224991	–2.635692	0.000000
C	0.306252	4.436720	0.000000
H	2.234362	3.844180	0.000000
H	0.734202	5.450563	0.000000

O	–0.883890	4.226032	0.000000
H	1.766389	–2.575589	–0.878032
H	1.766389	–2.575589	0.878032

Sum of electronic and thermal free energy: –531.406181 a.u.
N_{Im}= 0

22

	X	Y	Z
N	–1.098529	0.791955	0.000000
C	–0.001978	0.004006	0.000000
N	–0.138809	–1.298955	0.000000
C	1.046261	–1.950012	0.000000
C	2.328736	–1.422607	0.000000
C	2.483456	–0.001381	0.000000
N	1.217073	0.630770	0.000000
O	3.494804	0.679352	0.000000
N	1.206119	–3.303046	0.000000
C	2.563023	–3.526478	0.000000
N	3.268775	–2.430494	0.000000
H	–2.000166	0.348433	0.000000
H	–1.049092	1.794581	0.000000
C	0.145502	–4.292710	0.000000
H	2.959984	–4.531590	0.000000
H	1.257684	1.640812	0.000000
H	0.595944	–5.284065	0.000000
H	–0.475213	–4.178481	0.889211
H	–0.475213	–4.178481	–0.889211

Sum of electronic and thermal free energy: –581.745257 a.u.
N_{Im}= 1 (255*i* cm^{-1})

23

	X	Y	Z
C	0.059612	2.759293	0.000000
C	1.217033	1.931890	0.000000
N	1.205426	0.630185	0.000000
C	–0.001356	–0.000225	0.000000
C	–1.219472	0.724388	0.000000
C	–1.151487	2.144284	0.000000
O	2.402648	2.560684	0.000000
N	0.030572	–1.353008	0.000000
C	–2.427700	0.000858	0.000000
H	–2.069297	2.722274	0.000000
H	0.170355	3.835339	0.000000
H	–3.372436	0.534506	0.000000
C	–2.381454	–1.368521	0.000000
H	–3.282247	–1.968791	0.000000
C	–1.119017	–1.993110	0.000000
H	–1.061108	–3.078539	0.000000
H	3.091337	1.885414	0.000000

Sum of electronic and thermal free energy: –493.069338 a.u.

N_{Im}= 0

24

	X	Y	Z
N	–0.039901	1.354534	0.000000
C	–1.206720	2.120632	0.000000
C	–0.001047	–0.001750	0.000000
N	–1.052104	3.395347	0.000000
C	–2.453995	1.352301	0.000000
C	–2.399821	0.001628	0.000000
C	–1.169440	–0.733896	0.000000
N	1.216064	–0.610056	0.000000
C	1.307632	–1.977397	0.000000
H	2.058853	–0.055956	0.000000
C	–3.743225	2.117034	0.000000
H	–3.314696	–0.581497	0.000000
C	–1.130063	–2.189782	0.000000
H	–3.823418	2.760237	0.882696
H	–3.823418	2.760237	–0.882696
H	–4.593720	1.434895	0.000000
H	–1.951169	3.865163	0.000000
H	2.315428	–2.369967	0.000000
C	0.210789	–2.760926	0.000000
O	–2.151071	–2.884569	0.000000
H	0.315073	–3.837693	0.000000
H	0.817910	1.888251	0.000000

Sum of electronic and thermal free energy: –493.069338 a.u.
N_{Im}= 1 (344*i* cm^{-1})

25

	X	Y	Z
C	0.186587	–1.453089	0.000000
C	1.480670	–2.031441	0.000000
N	2.635404	–1.295107	0.000000
C	2.491511	0.004070	0.000000
C	1.272352	0.745467	0.000000
C	0.010346	–0.001023	0.000000
N	1.650744	–3.369241	0.000000
N	3.650300	0.754871	0.000000
C	1.315747	2.125829	0.000000
O	–1.087513	0.553402	0.000000
C	–0.921287	–2.306734	0.000000
C	0.587434	–4.160287	0.000000
C	0.854546	–5.639439	0.000000
C	–0.730849	–3.667469	0.000000
C	3.707341	2.101098	0.000000
C	5.065001	2.724062	0.000000
C	2.527897	2.817486	0.000000
H	–0.070747	–6.217002	0.000000
H	1.441110	–5.912376	–0.880540

H	1.441110	–5.912376	0.880540
H	4.985565	3.809474	0.000000
H	5.627273	2.413544	0.884262
H	5.627273	2.413544	–0.884262
H	0.374395	2.664922	0.000000
H	2.560402	3.897689	0.000000
H	–1.913995	–1.870642	0.000000
H	–1.568679	–4.353606	0.000000
H	4.508223	0.215211	0.000000

Sum of electronic and thermal free energy: –741.289866 a.u.
N_{Im}= 0

26

	X	Y	Z
N	–0.005392	0.005200	0.000000
C	–0.013790	–1.346096	0.000000
C	1.192281	0.740989	0.000000
N	–1.188782	–1.984871	0.000000
N	1.108556	–2.044972	0.000000
C	2.234410	–1.298146	0.000000
N	2.357224	–0.000862	0.000000
N	1.099842	2.013463	0.000000
H	3.158885	–1.870949	0.000000
H	2.037056	2.406527	0.000000
H	–0.861735	0.542175	0.000000
H	–1.178926	–2.990627	0.000000
H	–2.071150	–1.504401	0.000000

Sum of electronic and thermal free energy: –391.017703 a.u.
N_{Im}= 1 (104*i* cm^{-1})

27

	X	Y	Z
C	–0.112790	1.386965	0.000000
N	0.007774	–0.006888	0.000000
C	1.166886	–0.751755	0.000000
N	2.312897	0.015372	0.000000
C	2.303502	1.384777	0.000000
C	1.158210	2.087886	0.000000
O	–1.214473	1.903491	0.000000
O	1.181993	–1.964859	0.000000
H	3.278413	1.854103	0.000000
H	1.155146	3.166965	0.000000
H	–0.853939	–0.536584	0.000000
H	3.184211	–0.492073	0.000000

Sum of electronic and thermal free energy: –414.759028 a.u.
N_{Im}= 0

28

	X	Y	Z
N	3.672265	1.945283	0.000000

C	2.466646	1.346428	0.000000
N	2.406865	0.014375	0.000000
C	1.193989	–0.580243	0.000000
N	–0.006851	0.009020	0.000000
C	0.097311	1.339603	0.000000
C	1.267523	2.085051	0.000000
N	1.210649	–1.938001	0.000000
N	0.997148	3.442653	0.000000
C	–0.304069	3.506956	0.000000
N	–0.906279	2.270417	0.000000
H	0.346065	–2.447573	0.000000
H	2.088062	–2.424638	0.000000
H	3.741980	2.947664	0.000000
H	4.507223	1.385634	0.000000
H	–0.887302	4.415706	0.000000
H	–1.895904	2.083124	0.000000

Sum of electronic and thermal free energy: –522.580960 a.u.
N_{Im}= 1 (276*i* cm^{-1})

29

	X	Y	Z
N	–1.532935	–1.746905	0.000000
C	–0.252558	–1.353906	0.000000
N	0.006945	–0.038088	0.000000
C	1.285128	0.339336	0.000000
C	2.437305	–0.508723	0.000000
C	2.130752	–1.905557	0.000000
C	0.793666	–2.311137	0.000000
N	1.513874	1.683164	0.000000
H	0.687491	2.269011	0.000000
H	–1.750076	–2.729412	0.000000
H	–2.273121	–1.066262	0.000000
C	3.697976	0.066279	0.000000
C	2.735316	2.246969	0.000000
H	2.763042	3.327260	0.000000
C	3.855630	1.454013	0.000000
H	4.834935	1.910760	0.000000
H	4.564837	–0.584447	0.000000
N	0.733313	–3.672315	0.000000
N	2.926606	–2.994976	0.000000
C	2.028621	–4.006287	0.000000
H	2.348722	–5.041356	0.000000

Sum of electronic and thermal free energy: –620.783951 a.u.
N_{Im}= 0

30

	X	Y	Z
C	0.112936	1.737994	0.000000
O	0.090538	2.950358	0.000000
N	–1.065723	0.996800	0.000000

C	–1.220971	–0.373966	0.000000
O	–2.308324	–0.911264	0.000000
N	–0.033970	–1.084779	0.000000
C	1.177164	–0.449938	0.000000
C	1.298218	0.891111	0.000000
C	–0.128384	–2.544160	0.000000
H	2.046272	–1.094572	0.000000
Cl	2.851173	1.653415	0.000000
H	–1.926494	1.528544	0.000000
H	0.878313	–2.955982	0.000000
H	–0.661620	–2.882890	0.887835
H	–0.661620	–2.882890	–0.887835

Sum of electronic and thermal free energy: –913.649061 a.u.
N_{Im}= 0

31

	X	Y	Z
C	–0.002782	0.001106	0.000000
N	1.103674	–0.750112	0.000000
C	2.208235	0.000798	0.000000
C	2.276511	1.386735	0.000000
C	1.041029	2.061610	0.000000
N	–0.086753	1.349294	0.000000
N	3.589597	1.819042	0.000000
C	4.281871	0.713311	0.000000
N	3.509013	–0.424424	0.000000
N	–1.191458	–0.656521	0.000000
N	0.962286	3.405940	0.000000
H	–1.206454	–1.659933	0.000000
H	–2.048458	–0.134841	0.000000
H	1.798013	3.963707	0.000000
H	0.062088	3.853027	0.000000
C	3.961539	–1.801330	0.000000
H	5.360872	0.649663	0.000000
H	5.050710	–1.811799	0.000000
H	3.596608	–2.317578	0.888800
H	3.596608	–2.317578	–0.888800

Sum of electronic and thermal free energy: –561.863125 a.u.
N_{Im}= 2 (280*i* cm^{-1}, 19*i* cm^{-1})

32

	X	Y	Z
C	–1.119403	–2.130826	0.000000
N	–2.283045	–1.392636	0.000000
C	–2.417824	–0.003195	0.000000
C	–1.150489	0.695270	0.000000
C	–0.002924	–0.007795	0.000000
N	0.041112	–1.377033	0.000000
O	–1.111905	–3.345527	0.000000
O	–3.524331	0.506502	0.000000

C	1.307924	–2.104438	0.000000
H	0.962731	0.481684	0.000000
H	–1.148090	1.774437	0.000000
H	–3.138050	–1.933001	0.000000
H	2.121229	–1.381891	0.000000
H	1.379498	–2.733330	0.887269
H	1.379498	–2.733330	–0.887269

Sum of electronic and thermal free energy: –454.039274 a.u.
N_{Im}= 0

33

	X	Y	Z
O	–0.835006	–2.847205	0.000000
C	–1.604991	–1.910532	0.000000
N	–1.269264	–0.590632	0.000000
C	0.001424	0.001197	0.000000
C	1.179336	–0.724987	0.000000
C	2.373577	0.000265	0.000000
C	2.351924	1.393652	0.000000
C	1.097504	1.997594	0.000000
N	–0.054062	1.336170	0.000000
N	0.927479	3.389433	0.000000
C	1.867091	4.375279	0.000000
O	3.070463	4.221792	0.000000
O	3.499076	–0.726584	0.000000
H	–0.040484	3.678537	0.000000
H	–2.028136	0.076137	0.000000
C	4.749869	–0.048952	0.000000
H	5.507343	–0.829182	0.000000
H	4.860105	0.569393	–0.894952
H	4.860105	0.569393	0.894952
H	–2.697923	–2.045071	0.000000
H	1.400880	5.372706	0.000000
H	1.184051	–1.803262	0.000000
H	3.241309	2.000948	0.000000

Sum of electronic and thermal free energy: –700.060403 a.u.
N_{Im}= 0

34

	X	Y	Z
O	–1.086133	–1.990759	0.000000
C	–1.158404	–0.773678	0.000000
N	0.000316	–0.001955	0.000000
C	0.102838	1.372633	0.000000
O	1.173187	1.950933	0.000000
N	–1.107193	2.031349	0.000000
C	–2.297326	1.341503	0.000000
C	–2.392944	–0.001998	0.000000
C	–1.074385	3.491196	0.000000
H	–3.181168	1.967850	0.000000

C	–3.698044	–0.736562	0.000000
H	0.879017	–0.502686	0.000000
H	–2.098141	3.859557	0.000000
H	–0.556828	3.856266	0.887239
H	–0.556828	3.856266	–0.887239
H	–4.536940	–0.038603	0.000000
H	–3.781287	–1.380186	–0.879399
H	–3.781287	–1.380186	0.879399

Sum of electronic and thermal free energy: –493.329897 a.u.
N_{Im}= 0

35

	X	Y	Z
O	–0.897620	–4.156556	0.000000
C	–1.642850	–3.200170	0.000000
N	–1.272617	–1.888982	0.000000
C	0.013884	–1.332512	0.000000
N	0.003378	–0.001970	0.000000
C	1.166676	0.643932	0.000000
C	2.401447	–0.002502	0.000000
C	2.381948	–1.389308	0.000000
C	1.184448	–2.089028	0.000000
N	1.017672	2.037683	0.000000
C	1.976680	3.005459	0.000000
O	3.176023	2.827642	0.000000
H	0.055621	2.346375	0.000000
H	–2.014940	–1.203571	0.000000
H	–2.738825	–3.306070	0.000000
H	1.145656	–3.166671	0.000000
H	3.320347	0.561804	0.000000
H	1.529291	4.011550	0.000000
H	3.318170	–1.935375	0.000000

Sum of electronic and thermal free energy: –585.562680 a.u.
N_{Im}= 0

36

	X	Y	Z
O	0.726959	2.320112	0.000000
C	1.482637	1.224373	0.000000
C	2.877162	1.319353	0.000000
C	3.541192	0.092054	0.000000
N	2.990428	–1.120194	0.000000
C	1.656397	–1.069375	0.000000
N	0.888097	0.046038	0.000000
N	0.985611	–2.245795	0.000000
N	3.777928	2.371214	0.000000
C	4.941914	1.790415	0.000000
N	4.868124	0.416145	0.000000
H	5.641215	–0.229612	0.000000
H	5.894308	2.299562	0.000000

H	–0.196292	2.039897	0.000000
H	1.495507	–3.110512	0.000000
H	–0.017917	–2.249015	0.000000

Sum of electronic and thermal free energy: –542.453911 a.u.
N_{Im}= 1 (231*i* cm^{-1})

37

	X	Y	Z
C	–4.296423	0.767455	0.000000
C	–3.138342	–0.124264	0.000000
N	–1.915401	0.518694	0.000000
C	–1.726377	1.880310	0.000000
C	–2.853978	2.719616	0.000000
C	–4.156339	2.106390	0.000000
O	–3.204511	–1.345914	0.000000
N	–0.466459	2.315734	0.000000
C	–2.622780	4.096866	0.000000
H	–5.029359	2.750649	0.000000
H	–5.267444	0.289951	0.000000
H	–3.464297	4.781378	0.000000
C	–1.322346	4.563713	0.000000
H	–1.101831	5.623008	0.000000
C	–0.283633	3.631377	0.000000
H	–1.087649	–0.063571	0.000000
H	0.749169	3.965858	0.000000

Sum of electronic and thermal free energy: –493.084526 a.u.
N_{Im}= 0

38

	X	Y	Z
N	–0.631533	1.178470	0.000000
C	–1.960544	1.183537	0.000000
C	–0.013543	–0.006019	0.000000
N	–2.560748	2.399264	0.000000
C	–2.753149	–0.008452	0.000000
C	–2.075315	–1.196589	0.000000
C	–0.667528	–1.240437	0.000000
N	1.359325	0.023696	0.000000
C	2.094443	–1.119420	0.000000
H	1.805897	0.927901	0.000000
C	–4.252662	0.073241	0.000000
H	–2.613675	–2.138598	0.000000
C	0.078829	–2.501694	0.000000
H	–4.690012	–0.925525	0.000000
H	–3.558803	2.500926	0.000000
H	–1.988440	3.225585	0.000000
H	3.167873	–0.980211	0.000000
C	1.521685	–2.346326	0.000000
O	–0.481780	–3.602819	0.000000
H	2.141606	–3.232966	0.000000

H	–4.626333	0.600338	0.884585
H	–4.626333	0.600338	–0.884585

Sum of electronic and thermal free energy: –587.725668 a.u.
N_{Im}= 1 (219*i* cm^{-1})

39

	X	Y	Z
N	1.217143	0.482908	0.000000
C	–0.009738	–0.002848	0.000000
C	–1.281289	0.687828	0.000000
C	–2.443362	–0.005596	0.000000
C	–2.464196	–1.436495	0.000000
C	–1.231287	–2.107872	0.000000
N	–0.080511	–1.364340	0.000000
C	–3.620599	–2.227426	0.000000
C	–3.493029	–3.599300	0.000000
C	–2.206129	–4.151510	0.000000
N	–1.091487	–3.435546	0.000000
C	1.466786	1.826502	0.000000
O	0.682379	2.764791	0.000000
H	–3.388787	0.526610	0.000000
H	–1.258654	1.765459	0.000000
H	2.551206	2.024980	0.000000
H	–4.595625	–1.752935	0.000000
H	–4.359328	–4.247454	0.000000
H	–2.077814	–5.229425	0.000000
H	0.800411	–1.864841	0.000000

Sum of electronic and thermal free energy: –586.500091 a.u.
N_{Im}= 1 (32*i* cm^{-1})

40

	X	Y	Z
N	–1.277546	–0.576787	0.000000
C	0.001899	–0.000469	0.000000
C	1.184531	–0.724662	0.000000
C	2.373109	0.003764	0.000000
C	2.380682	1.387888	0.000000
C	1.114921	1.991207	0.000000
N	–0.030483	1.336132	0.000000
O	1.055832	3.337739	0.000000
C	–1.625913	–1.891814	0.000000
O	–0.864514	–2.836659	0.000000
C	3.633762	2.213519	0.000000
H	3.317818	–0.530252	0.000000
H	1.174326	–1.802884	0.000000
H	4.515926	1.571360	0.000000
H	3.678893	2.861414	–0.879532
H	3.678893	2.861414	0.879532
H	–2.030267	0.096837	0.000000
H	–2.720130	–2.016404	0.000000

H	0.126192	3.589785	0.000000

Sum of electronic and thermal free energy: –531.408829 a.u.
N_{Im}= 0

41

	X	Y	Z
C	1.121975	2.121167	0.000000
C	–0.062766	1.366839	0.000000
N	–0.001911	–0.001149	0.000000
C	1.178960	–0.694429	0.000000
C	2.399618	0.000277	0.000000
C	2.438704	1.469099	0.000000
N	–1.286354	1.901638	0.000000
N	1.079746	–2.026095	0.000000
C	3.564044	–0.770733	0.000000
O	3.488541	2.101530	0.000000
H	–0.867206	–0.522410	0.000000
C	0.984718	3.510953	0.000000
C	–1.394229	3.227467	0.000000
C	–2.787857	3.783286	0.000000
C	–0.272721	4.072764	0.000000
C	2.201370	–2.741234	0.000000
C	2.041251	–4.233044	0.000000
C	3.472886	–2.144951	0.000000
H	–2.785675	4.873522	0.000000
H	–3.329617	3.430338	–0.880772
H	–3.329617	3.430338	0.880772
H	3.006053	–4.740759	0.000000
H	1.475987	–4.546976	0.880772
H	1.475987	–4.546976	–0.880772
H	4.522277	–0.264014	0.000000
H	4.360466	–2.764595	0.000000
H	1.880603	4.121171	0.000000
H	–0.405583	5.147057	0.000000

Sum of electronic and thermal free energy: –741.308974 a.u.
N_{Im}= 0

42

	X	Y	Z
N	–0.003616	–0.002076	0.000000
C	–1.188582	0.614834	0.000000
N	–2.388846	–0.002235	0.000000
C	–2.308194	–1.324542	0.000000
N	–1.207235	–2.061352	0.000000
C	–0.068870	–1.336416	0.000000
N	1.089996	–2.017165	0.000000
N	–1.191614	1.958851	0.000000
H	1.963636	–1.521117	0.000000
H	–0.322536	2.462850	0.000000
H	–3.251268	–1.865718	0.000000

H	1.076055	–3.021647	0.000000
H	–2.065896	2.453632	0.000000

Sum of electronic and thermal free energy: –391.044314 a.u.
N_{Im}= 0

2. Quadruple hydrogen bonding monomers and complexes

3

	X	Y	Z
O	–1.05303	3.25138	0.00000
C	–1.09577	2.02462	0.00000
C	–2.35013	1.28443	0.00000
C	–2.35543	–0.06498	0.00000
N	–1.14727	–0.72155	0.00000
C	0.00517	–0.01196	0.00000
N	0.08159	1.28134	0.00000
N	1.19683	–0.71470	0.00000
C	1.36225	–2.09586	0.00000
O	0.41041	–2.87155	0.00000
N	2.64343	–2.50835	0.00000
H	3.39271	–1.83692	0.00000
H	2.00332	–0.10801	0.00000
H	–1.06440	–1.73735	0.00000
C	–3.58857	–0.91706	0.00000
H	–3.27868	1.83946	0.00000
C	2.97151	–3.92306	0.00000
H	–3.34427	–1.98003	0.00000
H	–4.19330	–0.70297	0.88284
H	–4.19330	–0.70297	–0.88284
H	4.05555	–4.02086	0.00000
H	2.57020	–4.41618	0.88738
H	2.57020	–4.41618	–0.88738

Sum of electronic and thermal free energy: –642.116441 a.u.
N_{Im} = 2 (151.38*i* cm^{-1}, 32.90*i* cm^{-1})

3•3

	X	Y	Z
O	–1.31568	1.84409	0.00000
C	–1.22960	0.60827	0.00000
C	–2.40944	–0.23119	0.00000
C	–2.27914	–1.57381	0.00000
N	–1.01376	–2.10388	0.00000
C	0.07761	–1.30630	0.00000
N	0.01200	0.00468	0.00000
N	1.30881	–1.89757	0.00000
C	1.55031	–3.28029	0.00000
O	0.63139	–4.10595	0.00000

N	2.84012	–3.61178	0.00000
H	3.57408	–2.89025	0.00000
H	2.10628	–1.24424	0.00000
H	–0.82300	–3.11110	0.00000
C	–3.40228	–2.55700	0.00000
H	–3.38259	0.23903	0.00000
O	4.95999	–1.84408	0.00000
C	4.87385	–0.60827	0.00000
C	6.05361	0.23133	0.00000
C	5.92315	1.57395	0.00000
N	4.65771	2.10386	0.00000
C	3.56646	1.30612	0.00000
N	3.63219	–0.00485	0.00000
N	2.33526	1.89732	0.00000
C	2.09400	3.28005	0.00000
O	3.01316	4.10544	0.00000
N	0.80424	3.61175	0.00000
H	0.07020	2.89031	0.00000
H	1.53774	1.24405	0.00000
H	4.46681	3.11105	0.00000
C	7.04618	2.55727	0.00000
H	7.02680	–0.23877	0.00000
C	3.24275	–5.00377	0.00000
C	0.40182	5.00379	0.00000
H	6.98947	3.19817	–0.88371
H	6.98947	3.19817	0.88371
H	8.00446	2.04058	0.00000
H	–0.68677	5.03728	0.00000
H	0.77308	5.52386	0.88637
H	0.77308	5.52386	–0.88637
H	4.33135	–5.03711	0.00000
H	2.87157	–5.52390	0.88637
H	2.87157	–5.52390	–0.88637
H	–3.34565	–3.19791	0.88371
H	–3.34565	–3.19791	–0.88371
H	–4.36051	–2.04020	0.00000

Sum of electronic and thermal free energy: –1284.269984 a.u.
$N_{Im} = 0$

43

	X	Y	Z
O	0.97853	–0.70732	0.00000
C	–0.06206	–0.06834	0.00000
N	–0.00686	1.33094	0.00000
C	–1.10751	2.11229	0.00000
C	–2.34473	1.55888	0.00000

C	–2.37978	0.13436	0.00000
N	–1.30674	–0.62803	0.00000
N	–3.55842	–0.58071	0.00000
H	–3.24299	2.15086	0.00000
H	–0.94244	3.18184	0.00000
H	0.91564	1.74073	0.00000
H	–3.40169	–1.57913	0.00000
C	–4.87052	–0.10854	0.00000
N	–5.79453	–1.10048	0.00000
O	–5.16390	1.07285	0.00000
H	–6.76352	–0.83310	0.00000
H	–5.56573	–2.07909	0.00000

Sum of electronic and thermal free energy: –563.550780 a.u.
N_{Im} = 1 (69.28*i* cm^{-1})

43•43

	X	Y	Z
O	–3.03768	1.94152	0.00000
C	–1.90337	2.42296	0.00000
N	–1.77891	3.80345	0.00000
C	–0.57862	4.42296	0.00000
C	0.56290	3.69920	0.00000
C	0.41895	2.27713	0.00000
N	–0.76849	1.67765	0.00000
N	1.49102	1.43310	0.00000
C	2.85409	1.79570	0.00000
O	3.23674	2.95617	0.00000
N	3.68306	0.74103	0.00000
H	3.38115	–0.23836	0.00000
H	1.25087	0.43700	0.00000
H	1.53256	4.16253	0.00000
H	–0.59141	5.50479	0.00000
H	–2.63873	4.33210	0.00000
O	3.03765	–1.94143	0.00000
C	1.90336	–2.42292	0.00000
N	1.77901	–3.80342	0.00000
C	0.57876	–4.42301	0.00000
C	–0.56281	–3.69934	0.00000
C	–0.41899	–2.27724	0.00000
N	0.76842	–1.67769	0.00000
N	–1.49108	–1.43320	0.00000
C	–2.85423	–1.79564	0.00000
O	–3.23705	–2.95605	0.00000
N	–3.68312	–0.74091	0.00000
H	–3.38118	0.23848	0.00000
H	–1.25087	–0.43712	0.00000

H	–1.53243	–4.16275	0.00000
H	0.59164	–5.50484	0.00000
H	2.63886	–4.33201	0.00000
H	–4.66673	–0.95030	0.00000
H	4.66666	0.95047	0.00000

Sum of electronic and thermal free energy: –1127.116679 a.u.
N_{Im} = 1 (23.18*i* cm^{-1})

44

	X	Y	Z
O	2.20029	4.01428	0.00000
C	2.17981	2.79647	0.00000
N	3.41023	2.09912	0.00000
C	3.50998	0.76525	0.00000
C	2.38014	–0.00041	0.00000
C	1.15847	0.72721	0.00000
N	1.04911	2.03633	0.00000
N	–0.00355	0.00860	0.00000
C	–0.03219	–1.36856	0.00000
C	1.12906	–2.10417	0.00000
N	–1.26390	–1.91917	0.00000
H	–0.86056	0.54360	0.00000
C	2.41447	–1.47991	0.00000
H	4.49981	0.32600	0.00000
H	4.24059	2.67512	0.00000
O	3.48947	–2.08644	0.00000
H	1.07259	–3.18439	0.00000
H	–1.36409	–2.91866	0.00000
H	–2.10129	–1.36370	0.00000

Sum of electronic and thermal free energy: –639.7287976 a.u.
N_{Im} = 1 (197.13*i* cm^{-1})

44•44

	X	Y	Z
O	4.33794	–3.04065	0.00000
O	–2.27757	0.08477	0.00000
C	3.24435	–3.60120	0.00000
C	–1.18397	0.64532	0.00000
N	3.20891	–4.99884	0.00000
N	–1.14853	2.04295	0.00000
C	2.06798	–5.70383	0.00000
C	–0.00761	2.74794	0.00000
C	0.86828	–5.05941	0.00000
C	1.19210	2.10352	0.00000
C	0.92665	–3.63845	0.00000
C	1.13373	0.68256	0.00000
N	2.05895	–2.94488	0.00000

N	0.00143	–0.01101	0.00000
N	–0.23324	–2.94414	0.00000
N	2.29361	–0.01175	0.00000
C	–1.46568	–3.57151	0.00000
C	3.52605	0.61562	0.00000
C	–1.56939	–4.94903	0.00000
C	3.62976	1.99314	0.00000
N	–2.52110	–2.74680	0.00000
N	4.58148	–0.20908	0.00000
H	–2.42618	–1.72846	0.00000
H	4.48656	–1.22742	0.00000
H	–0.17310	–1.91267	0.00000
H	2.23348	–1.04322	0.00000
C	–0.42317	–5.78920	0.00000
C	2.48355	2.83331	0.00000
H	2.13537	–6.78456	0.00000
H	–0.07500	3.82867	0.00000
H	4.10466	–5.46677	0.00000
H	–2.04428	2.51088	0.00000
O	–0.44049	–7.02535	0.00000
O	2.50086	4.06947	0.00000
H	–2.55211	–5.40195	0.00000
H	4.61249	2.44607	0.00000
H	–3.44437	–3.14354	0.00000
H	5.50475	0.18765	0.00000

Sum of electronic and thermal free energy: –1279.482635 a.u.
$N_{Im} = 0$

45

	X	Y	Z
H	3.43127	–3.04078	0.00000
N	3.55151	–2.03831	0.00000
C	2.34648	–1.36242	0.00000
N	1.27272	–2.08226	0.00000
C	0.07280	–1.40984	0.00000
C	0.00212	–0.00349	0.00000
C	1.23585	0.78166	0.00000
N	2.38125	–0.00184	0.00000
O	1.30790	1.99568	0.00000
C	–1.24689	0.61822	0.00000
N	–1.03300	–2.17322	0.00000
C	4.83083	–1.49295	0.00000
O	5.03268	–0.28607	0.00000
N	5.82289	–2.40684	0.00000
H	6.76926	–2.06675	0.00000
H	5.66734	–3.39993	0.00000

H	3.29895	0.44466	0.00000
H	–1.29924	1.70061	0.00000
C	–2.37644	–0.17031	0.00000
C	–2.20613	–1.55923	0.00000
H	–3.07837	–2.20725	0.00000
H	–3.37020	0.25794	0.00000

Sum of electronic and thermal free energy: –733.193648 a.u.
$N_{Im} = 0$

45•45

	X	Y	Z
N	1.64287	0.88466	0.00000
C	2.21886	–0.28791	0.00000
N	3.56657	–0.47634	0.00000
C	4.49620	0.54787	0.00000
C	3.88215	1.87276	0.00000
C	2.47948	1.97638	0.00000
O	5.68934	0.31639	0.00000
C	4.66032	3.02846	0.00000
N	1.88338	3.17994	0.00000
N	1.42913	–1.40723	0.00000
H	0.41819	–1.22780	0.00000
C	1.88842	–2.73401	0.00000
N	0.91683	–3.64974	0.00000
O	3.08579	–3.01707	0.00000
H	–0.41815	1.22779	0.00000
N	–1.42909	1.40720	0.00000
C	–2.21883	0.28789	0.00000
N	–1.64285	–0.88467	0.00000
C	–2.47948	–1.97638	0.00000
C	–3.88215	–1.87275	0.00000
C	–4.49618	–0.54785	0.00000
N	–3.56654	0.47635	0.00000
O	–5.68932	–0.31634	0.00000
C	–4.66032	–3.02844	0.00000
N	–1.88338	–3.17995	0.00000
H	–0.08864	–3.42380	0.00000
H	3.88126	–1.45269	0.00000
C	4.03273	4.25644	0.00000
H	5.73993	2.93493	0.00000
C	2.63846	4.27014	0.00000
H	4.58949	5.18369	0.00000
H	2.10371	5.21573	0.00000
C	–1.88842	2.73396	0.00000
O	–3.08580	3.01697	0.00000
N	–0.91685	3.64971	0.00000

H	–1.21382	4.61104	0.00000
H	0.08863	3.42379	0.00000
H	–3.88121	1.45271	0.00000
H	–5.73994	–2.93490	0.00000
C	–4.03274	–4.25643	0.00000
H	1.21379	–4.61107	0.00000
C	–2.63847	–4.27014	0.00000
H	–2.10373	–5.21573	0.00000
H	–4.58951	–5.18367	0.00000

Sum of electronic and thermal free energy: –1466.404621 a.u.
N_{Im} = 1 (9.80*i* cm^{-1})

46

	X	Y	Z
N	1.27836	–2.08507	0.00000
C	2.35219	–1.34695	0.00000
N	2.38441	0.00061	0.00000
C	1.20320	0.71561	0.00000
C	0.00491	0.00075	0.00000
C	0.03721	–1.48153	0.00000
N	1.29674	2.04248	0.00000
O	–0.99070	–2.14032	0.00000
N	3.55395	–2.02304	0.00000
H	3.43213	–3.02511	0.00000
C	4.83412	–1.47639	0.00000
N	5.82522	–2.39061	0.00000
O	5.03240	–0.26940	0.00000
H	5.66790	–3.38374	0.00000
H	3.28961	0.46888	0.00000
H	6.77220	–2.05200	0.00000
C	–1.17830	0.73537	0.00000
H	–2.12489	0.20807	0.00000
C	–1.10807	2.11618	0.00000
H	–2.00075	2.72780	0.00000
C	0.15135	2.71712	0.00000
H	0.23995	3.79903	0.00000

Sum of electronic and thermal free energy: –733.190728 a.u.
N_{Im} = 0

46•46

	X	Y	Z
N	1.06661	–1.47013	0.00000
N	–1.06661	1.47012	0.00000
C	–0.02850	–2.20872	0.00000
C	0.02851	2.20871	0.00000
N	–0.03332	–3.55461	0.00000
N	0.03333	3.55460	0.00000

C	1.14302	–4.27002	0.00000
C	–1.14301	4.27001	0.00000
C	2.33921	–3.55671	0.00000
C	–2.33919	3.55671	0.00000
C	2.29054	–2.08602	0.00000
C	–2.29053	2.08601	0.00000
N	1.05119	–5.59754	0.00000
N	–1.05117	5.59753	0.00000
O	3.33304	–1.42968	0.00000
O	–3.33303	1.42967	0.00000
N	–1.22855	–1.56080	0.00000
N	1.22856	1.56078	0.00000
H	–1.16771	–0.53282	0.00000
H	1.16772	0.53281	0.00000
C	–2.48979	–2.18057	0.00000
C	2.48979	2.18056	0.00000
N	–3.51666	–1.32837	0.00000
N	3.51667	1.32837	0.00000
O	–2.61592	–3.40424	0.00000
O	2.61591	3.40423	0.00000
H	–3.41270	–0.30665	0.00000
H	3.41271	0.30665	0.00000
H	–0.94769	–4.01682	0.00000
H	0.94770	4.01680	0.00000
H	–4.43713	–1.73450	0.00000
H	4.43714	1.73449	0.00000
C	3.52719	–4.28560	0.00000
C	–3.52717	4.28560	0.00000
H	4.47245	–3.75663	0.00000
H	–4.47244	3.75663	0.00000
C	3.45791	–5.66517	0.00000
C	–3.45789	5.66517	0.00000
H	4.35088	–6.27615	0.00000
H	–4.35086	6.27615	0.00000
C	2.19788	–6.26830	0.00000
C	–2.19786	6.26829	0.00000
H	2.11229	–7.35043	0.00000
H	–2.11227	7.35042	0.00000

Sum of electronic and thermal free energy: –1466.402916 a.u.
$N_{Im} = 1$ (4.54*i* cm^{-1})

45•46

	X	Y	Z
N	1.70713	–0.55815	0.00000
C	0.61599	–1.30054	0.00000
N	0.61492	–2.64627	0.00000

C	1.79294	–3.35863	0.00000
C	2.98680	–2.64208	0.00000
C	2.93355	–1.17152	0.00000
N	1.70394	–4.68636	0.00000
O	3.97402	–0.51307	0.00000
N	–0.58928	–0.65864	0.00000
H	–0.53820	0.36811	0.00000
C	–1.84538	–1.28859	0.00000
N	–2.87910	–0.44471	0.00000
O	–1.96339	–2.51285	0.00000
H	–2.78226	0.58153	0.00000
H	–0.29785	–3.11170	0.00000
C	4.17682	–3.36801	0.00000
H	5.12101	–2.83715	0.00000
C	4.11080	–4.74771	0.00000
H	5.00521	–5.35658	0.00000
C	2.85227	–5.35416	0.00000
H	2.76956	–6.43650	0.00000
H	1.79503	1.46385	0.00000
N	1.85733	2.49045	0.00000
C	0.65451	3.14262	0.00000
N	–0.44247	2.43123	0.00000
C	–1.62572	3.13118	0.00000
C	–1.68951	4.53635	0.00000
C	–0.44683	5.30392	0.00000
N	0.68102	4.50330	0.00000
O	–0.36014	6.51621	0.00000
C	–2.92957	5.17124	0.00000
N	–2.75004	2.39563	0.00000
C	3.12219	3.09995	0.00000
O	3.26348	4.32256	0.00000
N	4.14395	2.24093	0.00000
H	4.03721	1.21983	0.00000
H	1.61378	4.93087	0.00000
H	–2.96514	6.25438	0.00000
C	–4.07431	4.40193	0.00000
C	–3.92228	3.01594	0.00000
H	–4.79729	2.37195	0.00000
H	–5.06114	4.84466	0.00000
H	5.06603	2.64329	0.00000
H	–3.79462	–0.86207	0.00000

Sum of electronic and thermal free energy: –1466.404123 a.u.
N_{Im} = 1 (15.98*i* cm^{-1})

4

	X	Y	Z
N	1.25555	–2.10062	0.00000
C	0.10464	–1.45175	0.00000
C	0.00325	–0.02683	0.00000
C	1.15597	0.69698	0.00000
C	2.40468	0.03443	0.00000
C	2.40468	–1.38431	0.00000
N	3.55380	–2.10062	0.00000
C	4.70471	–1.45175	0.00000
C	4.80610	–0.02683	0.00000
C	3.65338	0.69698	0.00000
N	5.83958	–2.20124	0.00000
H	–0.96933	0.45023	0.00000
H	1.12762	1.78218	0.00000
N	–1.03023	–2.20124	0.00000
H	3.68173	1.78218	0.00000
H	5.77868	0.45023	0.00000
H	–0.95329	–3.20333	0.00000
H	5.76264	–3.20333	0.00000
H	6.74996	–1.77951	0.00000
H	–1.94061	–1.77951	0.00000

Sum of electronic and thermal free energy: –528.550869 a.u.
N_{Im} = 2 (265.87*i* cm^{-1}, 262.79*i* cm^{-1})

5

	X	Y	Z
N	2.09740	–1.13508	0.00000
C	2.73858	0.07839	0.00000
N	2.12106	1.21361	0.00000
C	0.74408	1.20133	0.00000
C	0.00725	0.00391	0.00000
C	0.71390	–1.27547	0.00000
N	0.14745	2.40231	0.00000
O	0.20285	–2.37732	0.00000
N	4.10662	0.00319	0.00000
H	4.53780	–0.90897	0.00000
C	5.07729	1.03075	0.00000
O	6.25087	0.70034	0.00000
N	4.62114	2.28992	0.00000
C	–1.38658	0.06028	0.00000
H	–1.95599	–0.86168	0.00000
C	–1.99523	1.29663	0.00000
H	–3.07223	1.40039	0.00000
C	–1.17734	2.43119	0.00000
H	–1.62809	3.41962	0.00000
H	2.62480	–1.99831	0.00000

H	3.62276	2.47071	0.00000
H	5.30092	3.03083	0.00000

Sum of electronic and thermal free energy: –733.191719 a.u.
$N_{Im} = 0$

4•5

	X	Y	Z
N	–1.15326	2.43156	0.00000
C	–2.31177	3.09428	0.00000
C	–2.39456	4.52048	0.00000
C	–1.24153	5.23560	0.00000
C	0.00060	4.56471	0.00000
C	0.00290	3.14741	0.00000
N	1.15711	2.43172	0.00000
C	2.31486	3.09668	0.00000
C	2.39529	4.52423	0.00000
C	1.24214	5.23799	0.00000
N	3.45993	2.38925	0.00000
H	–3.36583	4.99944	0.00000
H	–1.26060	6.32086	0.00000
N	–3.45768	2.38552	0.00000
H	1.25957	6.32322	0.00000
H	3.36556	5.00519	0.00000
H	–3.44609	1.36792	0.00000
H	3.44677	1.36961	0.00000
N	–1.13371	–0.55258	0.00000
C	0.00033	–1.32588	0.00000
N	–0.01063	–2.62382	0.00000
C	–1.21675	–3.27253	0.00000
C	–2.42778	–2.56721	0.00000
C	–2.39678	–1.11050	0.00000
N	–1.17187	–4.61535	0.00000
O	–3.40386	–0.41478	0.00000
N	1.18274	–0.63200	0.00000
H	1.15168	0.40081	0.00000
C	2.48208	–1.16164	0.00000
O	3.43537	–0.38618	0.00000
N	2.63079	–2.49052	0.00000
C	–3.63178	–3.27328	0.00000
H	–4.56834	–2.72852	0.00000
C	–3.58392	–4.64987	0.00000
H	–4.48383	–5.25073	0.00000
C	–2.32588	–5.26449	0.00000
H	–2.25807	–6.34891	0.00000
H	–1.07787	0.48914	0.00000
H	1.81275	–3.09191	0.00000

H	3.57203	–2.84427	0.00000
H	4.34211	2.86880	0.00000
H	–4.33976	2.86504	0.00000

Sum of electronic and thermal free energy: –1261.757558 a.u.
N_{Im} = 2 (37.32*i* cm^{-1}, 18.68*i* cm^{-1})

6

	X	Y	Z
C	0.75327	0.00000	0.00000
N	–0.01469	1.14363	0.00000
N	–0.01469	–1.14363	0.00000
C	0.41091	2.47627	0.00000
C	0.41091	–2.47627	0.00000
C	1.74998	2.87748	0.00000
C	1.74998	–2.87748	0.00000
C	2.01007	4.23807	0.00000
C	2.01007	–4.23807	0.00000
N	–0.60823	3.33607	0.00000
N	–0.60823	–3.33607	0.00000
H	3.03731	4.58455	0.00000
H	3.03731	–4.58455	0.00000
C	0.95843	5.14763	0.00000
C	0.95843	–5.14763	0.00000
C	–0.33111	4.63960	0.00000
C	–0.33111	–4.63960	0.00000
H	–1.18915	5.30491	0.00000
H	–1.18915	–5.30491	0.00000
H	1.12990	6.21628	0.00000
H	1.12990	–6.21628	0.00000
H	2.54029	2.14375	0.00000
H	2.54029	–2.14375	0.00000
H	–1.02135	1.06562	0.00000
H	–1.02135	–1.06562	0.00000
O	1.97042	0.00000	0.00000

Sum of electronic and thermal free energy: –719.245853 a.u.
N_{Im} = 1 (25.80*i* cm^{-1})

4•6

	X	Y	Z
C	–0.01000	0.71473	0.00000
N	–1.19089	0.00284	0.00000
N	1.13138	–0.05890	0.00000
C	–2.46746	0.57985	0.00000
C	2.43681	0.44945	0.00000
C	–2.72956	1.95922	0.00000
C	2.77185	1.81294	0.00000
C	–4.04862	2.37686	0.00000

C	4.11124	2.15990	0.00000
N	–3.45903	–0.31150	0.00000
N	3.37961	–0.49333	0.00000
H	–4.26572	3.43910	0.00000
H	4.38448	3.20910	0.00000
C	–5.08160	1.44628	0.00000
C	5.09330	1.17573	0.00000
C	–4.72339	0.11172	0.00000
C	4.66468	–0.13790	0.00000
H	–5.48034	–0.66788	0.00000
H	5.37913	–0.95663	0.00000
H	–6.12234	1.74236	0.00000
H	6.14831	1.41610	0.00000
H	–1.92034	2.66774	0.00000
H	2.00142	2.56347	0.00000
H	–1.17616	–1.02249	0.00000
H	1.06219	–1.08201	0.00000
O	0.02242	1.93426	0.00000
N	1.03577	–3.34269	0.00000
C	2.17172	–4.03868	0.00000
C	2.22073	–5.46720	0.00000
C	1.04909	–6.15214	0.00000
C	–0.17384	–5.44689	0.00000
C	–0.13609	–4.02717	0.00000
N	–1.26991	–3.28138	0.00000
C	–2.44124	–3.91602	0.00000
C	–2.56609	–5.33992	0.00000
C	–1.43251	–6.08616	0.00000
N	–3.56248	–3.16721	0.00000
H	3.17954	–5.97111	0.00000
H	1.03808	–7.23769	0.00000
N	3.33116	–3.35051	0.00000
H	–1.47921	–7.17076	0.00000
H	–3.55033	–5.79217	0.00000
H	–3.48474	–2.14705	0.00000
H	3.30775	–2.32765	0.00000
H	4.20669	–3.84152	0.00000
H	–4.46286	–3.61100	0.00000

Sum of electronic and thermal free energy: –1247.797445 a.u.
N_{Im} = 5 (58.42*i* cm^{-1}, 48.69*i* cm^{-1}, 37.23*i* cm^{-1}, 34.40*i* cm^{-1}, 13.90*i* cm^{-1})

47

	X	Y	Z
N	1.26349	–2.06509	0.00000
C	0.12370	–1.41395	0.00000
C	0.00779	0.00088	0.00000

C	1.16435	0.72524	0.00000
C	2.41245	0.06487	0.00000
C	2.41245	–1.35068	0.00000
N	3.56141	–2.06509	0.00000
C	4.70121	–1.41395	0.00000
C	4.81711	0.00088	0.00000
C	3.66055	0.72524	0.00000
N	5.82233	–2.25193	0.00000
H	–0.96604	0.46488	0.00000
H	1.13341	1.80948	0.00000
N	–0.99742	–2.25193	0.00000
H	3.69149	1.80948	0.00000
H	5.79095	0.46488	0.00000
C	–2.32546	–1.93618	0.00000
H	–0.76287	–3.23535	0.00000
C	7.15037	–1.93618	0.00000
H	5.58777	–3.23535	0.00000
O	–2.80121	–0.82184	0.00000
O	7.62612	–0.82184	0.00000
H	7.77395	–2.84333	0.00000
H	–2.94905	–2.84333	0.00000

Sum of electronic and thermal free energy: –755.197649 a.u.
$N_{Im} = 0$

48

	X	Y	Z
O	1.33862	–2.01047	0.00000
C	–0.00329	–0.03320	0.00000
C	0.06129	1.32081	0.00000
H	–0.84775	1.91250	0.00000
N	1.21617	2.04913	0.00000
C	2.33341	1.37417	0.00000
N	2.36375	0.01393	0.00000
C	1.21646	–0.79720	0.00000
N	3.55068	1.99722	0.00000
C	3.88621	3.37500	0.00000
O	5.07380	3.65887	0.00000
N	2.86408	4.23846	0.00000
C	3.06161	5.67395	0.00000
H	4.12918	5.88474	0.00000
H	2.61165	6.12051	–0.88925
H	2.61165	6.12051	0.88925
H	4.38076	1.42343	0.00000
H	3.24490	–0.48392	0.00000
H	1.92812	3.84284	0.00000
H	–0.94470	–0.56338	0.00000

Sum of electronic and thermal free energy: –602.826495 a.u.
N_{Im} = 1 (64.84*i* cm^{-1})

47•48

	X	Y	Z
O	–3.36714	1.98130	0.00000
C	–2.20444	4.04522	0.00000
C	–0.97061	4.60666	0.00000
H	–0.85316	5.68496	0.00000
N	0.19174	3.90176	0.00000
C	0.09827	2.59627	0.00000
N	–1.09429	1.94413	0.00000
C	–2.31329	2.61799	0.00000
N	1.21212	1.80283	0.00000
C	2.56362	2.19101	0.00000
O	3.41516	1.30057	0.00000
N	2.84434	3.49401	0.00000
C	4.20283	3.99977	0.00000
H	4.89631	3.16180	0.00000
H	4.37922	4.60839	–0.88918
H	4.37922	4.60839	0.88918
H	1.07842	0.78483	0.00000
H	–1.13248	0.90983	0.00000
H	2.05037	4.12982	0.00000
N	–1.41568	–1.09104	0.00000
C	–2.62141	–1.64083	0.00000
C	–2.85422	–3.04102	0.00000
C	–1.77204	–3.86582	0.00000
C	–0.47231	–3.32069	0.00000
C	–0.33299	–1.91234	0.00000
N	0.88787	–1.31687	0.00000
C	1.96202	–2.09235	0.00000
C	1.91792	–3.51133	0.00000
C	0.69587	–4.10935	0.00000
N	3.17381	–1.41760	0.00000
C	4.44342	–1.91833	0.00000
O	4.77893	–3.08501	0.00000
N	–3.67883	–0.74300	0.00000
C	–5.02185	–0.98896	0.00000
O	–5.57600	–2.06882	0.00000
H	3.12568	–0.39024	0.00000
H	–3.43460	0.25642	0.00000
H	–3.86641	–3.41224	0.00000
H	–1.89867	–4.94311	0.00000
H	0.60964	–5.19045	0.00000
H	2.83829	–4.07292	0.00000

H	–3.11034	4.63345	0.00000
H	5.17852	–1.09887	0.00000
H	–5.58486	–0.04306	0.00000

Sum of electronic and thermal free energy: –1358.039054 a.u.
N_{Im} = 2 (79.62*i* cm^{-1}, 7.61*i* cm^{-1})

49

	X	Y	Z
O	5.87745	0.71712	0.00000
C	4.88788	–0.00029	0.00000
C	4.87615	–1.44623	0.00000
C	3.71081	–2.13708	0.00000
C	2.44491	–1.48119	0.00000
C	2.44491	–0.09593	0.00000
N	3.61586	0.59062	0.00000
N	1.27396	0.59062	0.00000
C	0.00194	–0.00029	0.00000
H	1.27328	1.60262	0.00000
H	3.61655	1.60262	0.00000
H	5.83809	–1.93994	0.00000
H	3.72433	–3.22214	0.00000
O	–0.98763	0.71712	0.00000
C	0.01367	–1.44623	0.00000
H	–0.94827	–1.93994	0.00000
C	1.17901	–2.13708	0.00000
H	1.16549	–3.22214	0.00000

Sum of electronic and thermal free energy: –568.323898 a.u.
N_{Im} = 1 (160.67*i* cm^{-1})

47•49

	X	Y	Z
O	–0.25340	–4.18105	0.00000
C	–1.24548	–3.44534	0.00000
C	–2.60796	–3.91153	0.00000
C	–3.64081	–3.03401	0.00000
C	–3.41999	–1.62866	0.00000
C	–2.10363	–1.18778	0.00000
N	–1.07377	–2.06923	0.00000
N	–1.81238	0.13613	0.00000
C	–2.77826	1.13123	0.00000
H	–0.82232	0.43963	0.00000
H	–0.10063	–1.71522	0.00000
H	–2.75766	–4.98223	0.00000
H	–4.66382	–3.39544	0.00000
N	1.03581	1.08462	0.00000
C	1.29906	2.38328	0.00000
C	2.61253	2.92198	0.00000

C	3.65830	2.05093	0.00000
C	3.41865	0.66176	0.00000
C	2.07790	0.21270	0.00000
N	1.77118	–1.11097	0.00000
C	2.76350	–1.98910	0.00000
C	4.13647	–1.62804	0.00000
C	4.44664	–0.30284	0.00000
N	2.37432	–3.32111	0.00000
H	2.74948	3.99134	0.00000
H	4.67977	2.41551	0.00000
N	0.18610	3.21216	0.00000
H	5.48165	0.02134	0.00000
H	4.88986	–2.39921	0.00000
O	–2.42939	2.31604	0.00000
C	–4.14669	0.68280	0.00000
H	–4.91105	1.44735	0.00000
C	–4.44267	–0.63978	0.00000
H	–5.47701	–0.96739	0.00000
C	0.12725	4.57724	0.00000
H	–0.73720	2.75715	0.00000
C	3.14959	–4.44621	0.00000
H	1.36324	–3.51401	0.00000
H	–0.92020	4.91550	0.00000
O	1.05705	5.35669	0.00000
H	2.51724	–5.34715	0.00000
O	4.36128	–4.50829	0.00000

Sum of electronic and thermal free energy: –1323.538273 a.u.
$N_{Im} = 1$ (15.79*i* cm^{-1})

4•48

	X	Y	Z
O	4.40474	3.09052	0.00000
C	4.67286	1.89010	0.00000
C	5.99841	1.34561	0.00000
C	6.15246	0.00000	0.00000
N	5.12318	–0.88576	0.00000
C	3.90611	–0.39665	0.00000
N	3.65184	0.93940	0.00000
N	2.81555	–1.22314	0.00000
C	2.79294	–2.63114	0.00000
O	1.69890	–3.19393	0.00000
N	3.96086	–3.28019	0.00000
C	4.04656	–4.72602	0.00000
H	3.04157	–5.14259	0.00000
H	4.57651	–5.07520	–0.88898
H	4.57651	–5.07520	0.88898

H	4.79914	–2.70340	0.00000
H	1.87598	–0.79449	0.00000
H	2.67343	1.29981	0.00000
H	6.83625	2.02744	0.00000
H	7.14177	–0.44550	0.00000
N	0.00000	0.00000	0.00000
C	–1.06609	–0.80317	0.00000
C	–2.41043	–0.31658	0.00000
C	–2.61342	1.02477	0.00000
C	–1.50666	1.90188	0.00000
C	–0.20420	1.34265	0.00000
N	0.90841	2.12335	0.00000
C	0.75629	3.44958	0.00000
C	–0.52315	4.08686	0.00000
C	–1.63423	3.30820	0.00000
N	1.85954	4.22142	0.00000
H	1.76658	5.22107	0.00000
H	–3.23403	–1.01999	0.00000
H	–3.61816	1.43539	0.00000
N	–0.86358	–2.13415	0.00000
H	–1.65023	–2.75791	0.00000
H	–2.62453	3.75269	0.00000
H	–0.58180	5.16838	0.00000
H	2.79230	3.80815	0.00000
H	0.08061	–2.51987	0.00000

Sum of electronic and thermal free energy: –1131.392018 a.u.
$N_{Im} = 3$ (92.71*i* cm^{-1}, 36.33*i* cm^{-1}, 17.84*i* cm^{-1})

4•49

	X	Y	Z
O	3.60427	–0.64631	0.00000
C	3.72888	0.58133	0.00000
C	4.99953	1.26190	0.00000
C	5.06105	2.61469	0.00000
C	3.88169	3.40850	0.00000
C	2.65779	2.74767	0.00000
N	2.60094	1.39166	0.00000
N	1.49276	3.44396	0.00000
C	1.43392	4.83161	0.00000
H	0.58468	2.93083	0.00000
H	1.67379	0.91382	0.00000
H	5.88483	0.64105	0.00000
H	6.02207	3.11875	0.00000
N	–1.09672	2.03157	0.00000
C	–2.22801	2.73986	0.00000
C	–3.52213	2.13306	0.00000

C	–3.60341	0.77840	0.00000
C	–2.42318	0.00248	0.00000
C	–1.17736	0.67542	0.00000
N	0.00111	–0.00059	0.00000
C	–0.02690	–1.33493	0.00000
C	–1.24382	–2.08457	0.00000
C	–2.42135	–1.41001	0.00000
N	1.14350	–2.00118	0.00000
H	1.14190	–3.00551	0.00000
H	–4.40574	2.75885	0.00000
H	–4.56747	0.27980	0.00000
N	–2.14287	4.08393	0.00000
H	–2.98294	4.63430	0.00000
H	–3.36691	–1.94290	0.00000
H	–1.20434	–3.16658	0.00000
H	2.03754	–1.50797	0.00000
H	–1.23994	4.56060	0.00000
O	0.33906	5.40071	0.00000
C	2.70003	5.52071	0.00000
H	2.66666	6.60151	0.00000
C	3.86486	4.83004	0.00000
H	4.81351	5.35702	0.00000

Sum of electronic and thermal free energy: –1096.892207 a.u.
N_{Im} = 2 (27.35*i* cm^{-1}, 15.95*i* cm^{-1})

50

	X	Y	Z
N	1.05569	1.99082	0.00000
C	1.17420	0.63261	0.00000
C	2.43400	0.00764	0.00000
C	2.46285	–1.37167	0.00000
C	1.28559	–2.11651	0.00000
C	0.09447	–1.39753	0.00000
N	0.03473	–0.06216	0.00000
N	–1.17810	–1.97665	0.00000
C	–1.51981	–3.31318	0.00000
O	–0.70946	–4.22660	0.00000
N	–2.86489	–3.53422	0.00000
H	–3.17765	–4.48892	0.00000
H	–3.55236	–2.80147	0.00000
H	–1.91490	–1.28742	0.00000
H	1.28185	–3.19405	0.00000
H	3.41662	–1.88812	0.00000
H	3.34290	0.59655	0.00000
H	1.86287	2.58626	0.00000
H	0.14070	2.40476	0.00000

Sum of electronic and thermal free energy: –527.605095 a.u.
N_{Im} = 2 (339.37*i* cm^{-1}, 249.43*i* cm^{-1})

51

	X	Y	Z
O	3.19693	–1.67147	0.00000
C	3.11182	–0.45550	0.00000
N	4.28388	0.31467	0.00000
C	4.27415	1.66064	0.00000
C	3.10144	2.34298	0.00000
C	1.91799	1.54886	0.00000
N	1.93338	0.23350	0.00000
N	0.63468	2.06511	0.00000
C	0.06814	3.33405	0.00000
O	–1.14369	3.40479	0.00000
C	0.93511	4.56138	0.00000
H	0.27823	5.42804	0.00000
H	1.56852	4.59337	0.88871
H	1.56852	4.59337	–0.88871
H	3.10906	3.41688	0.00000
H	5.23645	2.15509	0.00000
H	5.15559	–0.19501	0.00000
H	–0.06550	1.33211	0.00000

Sum of electronic and thermal free energy: –547.470694 a.u.
N_{Im} = 1 (45.91*i* cm^{-1})

50•51

	X	Y	Z
N	–3.32834	1.65734	0.00000
C	–3.25038	0.30236	0.00000
C	–4.42837	–0.46850	0.00000
C	–4.29992	–1.83827	0.00000
C	–3.04363	–2.43396	0.00000
C	–1.93370	–1.58929	0.00000
N	–2.02545	–0.24827	0.00000
N	–0.61918	–2.05951	0.00000
C	–0.20456	–3.38489	0.00000
O	–0.97317	–4.34038	0.00000
N	1.13849	–3.54434	0.00000
H	1.46985	–4.49303	0.00000
H	1.81897	–2.78622	0.00000
H	0.09245	–1.33411	0.00000
H	–2.91511	–3.50213	0.00000
H	–5.18529	–2.46527	0.00000
H	–5.39707	0.01608	0.00000
H	–4.22659	2.10461	0.00000
H	–2.49557	2.23283	0.00000

O	3.22840	–1.67120	0.00000
C	3.11247	–0.45148	0.00000
N	4.26794	0.32377	0.00000
C	4.23620	1.66790	0.00000
C	3.05050	2.32413	0.00000
C	1.87449	1.51900	0.00000
N	1.91554	0.19886	0.00000
N	0.59277	2.03157	0.00000
C	0.08631	3.32310	0.00000
O	–1.12275	3.45803	0.00000
C	0.97610	4.53372	0.00000
H	0.32644	5.40549	0.00000
H	1.60696	4.56130	0.88996
H	1.60696	4.56130	–0.88996
H	3.04859	3.39596	0.00000
H	5.18921	2.17964	0.00000
H	5.14529	–0.17686	0.00000
H	–0.13524	1.31047	0.00000

Sum of electronic and thermal free energy: –1075.074272 a.u.
N_{Im} = 4 (138.43*i* cm^{-1}, 44.72*i* cm^{-1}, 24.31*i* cm^{-1}, 13.86*i* cm^{-1})

52

	X	Y	Z
N	–3.26971	–1.75333	0.00000
C	–3.13663	–0.40309	0.00000
C	–4.27964	0.43619	0.00000
C	–4.08951	1.79230	0.00000
C	–2.79262	2.32818	0.00000
C	–1.74764	1.40497	0.00000
N	–1.89401	0.07817	0.00000
N	–0.44722	1.86021	0.00000
C	–0.14088	3.19178	0.00000
C	–1.13850	4.13811	0.00000
N	1.18045	3.49841	0.00000
H	1.89463	2.79260	0.00000
H	0.27726	1.15753	0.00000
C	–2.52408	3.77703	0.00000
H	–4.92990	2.47696	0.00000
H	–5.27175	0.00204	0.00000
O	–3.44913	4.60304	0.00000
H	–0.87293	5.18734	0.00000
H	1.46877	4.45991	0.00000
H	–2.44736	–2.33071	0.00000
H	–4.17344	–2.18967	0.00000

Sum of electronic and thermal free energy: –603.788122 a.u.
N_{Im} = 2 (312.67*i* cm^{-1}, 220.52*i* cm^{-1})

53

	X	Y	Z
O	2.61493	2.26458	0.00000
C	1.96563	1.23558	0.00000
N	2.65782	0.00104	0.00000
C	2.05517	–1.19357	0.00000
C	0.68961	–1.26197	0.00000
C	0.01554	0.00022	0.00000
N	0.60419	1.17225	0.00000
N	–1.34872	–0.02575	0.00000
C	–2.14657	–1.16893	0.00000
C	–1.42282	–2.43986	0.00000
O	–3.35923	–1.06406	0.00000
H	–1.82860	0.86596	0.00000
C	–0.07956	–2.47693	0.00000
H	2.69068	–2.07085	0.00000
H	3.66633	0.06484	0.00000
H	–2.02831	–3.33584	0.00000
H	0.44836	–3.42451	0.00000

Sum of electronic and thermal free energy: –584.382627 a.u.
$N_{Im} = 0$

52•53

	X	Y	Z
O	3.35315	1.60543	0.00000
N	–3.29819	–1.76135	0.00000
C	3.10564	0.40728	0.00000
C	–3.12995	–0.42117	0.00000
N	4.17821	–0.49759	0.00000
C	–4.26452	0.43118	0.00000
C	4.02278	–1.82648	0.00000
C	–4.06683	1.78285	0.00000
C	2.76523	–2.36300	0.00000
C	–2.76757	2.31002	0.00000
C	1.68773	–1.42303	0.00000
C	–1.71729	1.39062	0.00000
N	1.85156	–0.11344	0.00000
N	–1.87641	0.05420	0.00000
N	0.41800	–1.90392	0.00000
N	–0.42272	1.85036	0.00000
C	0.09088	–3.25426	0.00000
C	–0.13110	3.18746	0.00000
C	1.20285	–4.19860	0.00000
C	–1.13777	4.13114	0.00000
O	–1.08158	–3.60105	0.00000
N	1.18100	3.50764	0.00000

H	1.92192	2.81029	0.00000
H	–0.36375	–1.22058	0.00000
H	0.33806	1.16520	0.00000
C	2.47527	–3.77061	0.00000
C	–2.51337	3.76109	0.00000
H	4.92182	–2.42994	0.00000
H	–4.90083	2.47544	0.00000
H	5.10261	–0.08797	0.00000
H	–5.25835	0.00094	0.00000
O	–3.45305	4.57575	0.00000
H	0.94002	–5.24736	0.00000
H	–0.87655	5.18193	0.00000
H	1.43927	4.47782	0.00000
H	3.30040	–4.47437	0.00000
H	–2.50768	–2.39913	0.00000
H	–4.22589	–2.14543	0.00000

Sum of electronic and thermal free energy: –1188.181057 a.u.
N_{Im} = 2 (46.24*i* cm^{-1}, 29.42*i* cm^{-1})

54

	X	Y	Z
N	1.09057	2.01690	0.00000
C	1.18446	0.66473	0.00000
C	2.44199	0.00040	0.00000
C	2.45012	–1.40747	0.00000
C	1.26041	–2.08193	0.00000
C	0.06140	–1.31829	0.00000
N	0.01066	–0.01269	0.00000
N	–1.14097	–1.99794	0.00000
C	–1.27978	–3.36276	0.00000
C	1.20067	–3.55503	0.00000
H	3.38424	–1.95869	0.00000
C	3.61925	0.78299	0.00000
H	–1.99185	–1.45293	0.00000
O	–2.35458	–3.91940	0.00000
N	–0.08405	–4.06814	0.00000
O	2.17118	–4.28122	0.00000
H	–0.17508	–5.07555	0.00000
H	4.58660	0.29268	0.00000
C	3.50432	2.14362	0.00000
H	4.37243	2.78977	0.00000
C	2.20776	2.70654	0.00000
H	2.10030	3.78810	0.00000

Sum of electronic and thermal free energy: –754.034381 a.u.
N_{Im} = 0

50•54

	X	Y	Z
N	1.01825	4.87789	0.00000
C	2.29396	4.41683	0.00000
C	3.35995	5.33613	0.00000
C	4.64094	4.83830	0.00000
C	4.86813	3.46679	0.00000
C	3.75487	2.62844	0.00000
N	2.48671	3.08519	0.00000
N	3.85828	1.23661	0.00000
C	5.02821	0.48710	0.00000
O	6.15369	0.97255	0.00000
N	4.82736	–0.85123	0.00000
H	5.65908	–1.41563	0.00000
H	3.91883	–1.31724	0.00000
H	2.97729	0.72879	0.00000
H	5.86020	3.05148	0.00000
H	5.48673	5.51747	0.00000
H	3.15794	6.40003	0.00000
H	0.85498	5.86826	0.00000
H	0.21600	4.25987	0.00000
N	2.43050	–2.48948	0.00000
C	1.19059	–1.95017	0.00000
C	0.03323	–2.77066	0.00000
C	–1.22088	–2.13408	0.00000
C	–1.27399	–0.76947	0.00000
C	–0.05214	–0.03601	0.00000
N	1.13385	–0.59422	0.00000
N	–0.11140	1.34190	0.00000
C	–1.28187	2.05124	0.00000
C	–2.56747	–0.06545	0.00000
H	–2.14121	–2.70793	0.00000
C	0.19628	–4.17392	0.00000
H	0.77021	1.88098	0.00000
O	–1.32763	3.26626	0.00000
N	–2.44888	1.30912	0.00000
O	–3.64864	–0.61185	0.00000
H	–3.30395	1.84977	0.00000
H	–0.67983	–4.81271	0.00000
C	1.46004	–4.69414	0.00000
H	1.63894	–5.76102	0.00000
C	2.54846	–3.79806	0.00000
H	3.56345	–4.18561	0.00000

Sum of electronic and thermal free energy: –1281.644080 a.u.
N_{Im} = 2 (95.68*i* cm^{-1}, 25.97*i* cm^{-1})

55

	X	Y	Z
H	–0.90951	–3.09287	0.00000
N	–1.08142	–2.09631	0.00000
C	0.07552	–1.33116	0.00000
N	1.19159	–2.06239	0.00000
C	2.34335	–1.39857	0.00000
C	2.39682	–0.00253	0.00000
C	1.17107	0.63269	0.00000
N	–0.00082	–0.00695	0.00000
H	1.12036	1.71697	0.00000
H	3.33014	0.53572	0.00000
C	–2.42988	–1.77327	0.00000
O	–3.22874	–2.69167	0.00000
C	–2.85683	–0.33479	0.00000
H	–3.94482	–0.31126	0.00000
N	3.46134	–2.22399	0.00000
H	3.24525	–3.21146	0.00000
C	4.78572	–1.87450	0.00000
O	5.22228	–0.74700	0.00000
H	5.43335	–2.76420	0.00000
H	–2.46160	0.18366	0.87415
H	–2.46160	0.18366	–0.87415

Sum of electronic and thermal free energy: –640.914799 a.u.
$N_{Im} = 0$

55•55

	X	Y	Z
N	–2.00714	–0.00720	0.00000
C	–2.00689	1.32791	0.00000
N	–3.06613	2.12174	0.00000
C	–4.25044	1.50660	0.00000
C	–4.39676	0.13820	0.00000
C	–3.20794	–0.60032	0.00000
H	–5.12301	2.15226	0.00000
H	–5.36039	–0.34322	0.00000
N	–3.16942	–1.97905	0.00000
H	–2.23579	–2.40922	0.00000
C	–4.21937	–2.85572	0.00000
O	–5.39870	–2.57679	0.00000
N	–0.73695	1.90146	0.00000
H	0.04087	1.24151	0.00000
C	–0.35046	3.22101	0.00000
O	0.85129	3.46718	0.00000
C	–1.34898	4.33842	0.00000
H	–1.99767	4.27713	0.87353
H	–1.99767	4.27713	–0.87353

H	–0.79020	5.27223	0.00000
H	–0.04087	–1.24151	0.00000
N	0.73695	–1.90146	0.00000
C	2.00689	–1.32791	0.00000
N	2.00714	0.00720	0.00000
C	3.20794	0.60032	0.00000
C	4.39676	–0.13820	0.00000
C	4.25044	–1.50660	0.00000
N	3.06613	–2.12174	0.00000
H	5.12301	–2.15226	0.00000
H	5.36039	0.34322	0.00000
C	0.35046	–3.22101	0.00000
O	–0.85129	–3.46718	0.00000
C	1.34898	–4.33842	0.00000
H	0.79020	–5.27223	0.00000
H	1.99767	–4.27713	0.87353
H	1.99767	–4.27713	–0.87353
N	3.16942	1.97905	0.00000
H	2.23579	2.40922	0.00000
C	4.21937	2.85572	0.00000
O	5.39870	2.57679	0.00000
H	–3.85867	–3.89533	0.00000
H	3.85867	3.89533	0.00000

Sum of electronic and thermal free energy: –1281.833760 a.u.
N_{Im} = 2 (49.68*i* cm^{-1}, 48.28*i* cm^{-1})

56

	X	Y	Z
H	–0.97114	1.77688	0.00000
N	–1.13607	0.78167	0.00000
C	0.00042	0.00425	0.00000
N	1.14054	0.69771	0.00000
C	2.27284	–0.00023	0.00000
C	2.28276	–1.40056	0.00000
C	1.04181	–1.99956	0.00000
N	–0.11106	–1.32348	0.00000
H	0.95756	–3.08146	0.00000
H	3.19973	–1.96504	0.00000
C	–2.50012	0.45050	0.00000
O	–3.31972	1.36048	0.00000
N	–2.81483	–0.85385	0.00000
H	–2.05061	–1.52076	0.00000
C	–4.19840	–1.28160	0.00000
H	–4.72446	–0.91795	0.88583
H	–4.72446	–0.91795	–0.88583
H	–4.21894	–2.37049	0.00000

N	3.40863	0.79292	0.00000
H	3.20600	1.78295	0.00000
C	4.73716	0.41145	0.00000
O	5.09415	–0.74776	0.00000
C	5.69340	1.57760	0.00000
H	5.53404	2.19972	0.88415
H	5.53404	2.19972	–0.88415
H	6.71326	1.20055	0.00000

Sum of electronic and thermal free energy: –735.571510 a.u.
$N_{Im} = 0$

56•56

	X	Y	Z
N	0.08561	–2.01134	0.00000
C	–1.25040	–1.99761	0.00000
N	–2.04800	–3.06316	0.00000
C	–1.43798	–4.25173	0.00000
C	–0.07358	–4.40203	0.00000
C	0.67625	–3.21504	0.00000
H	–2.08822	–5.12054	0.00000
H	0.40284	–5.36701	0.00000
N	2.05121	–3.18213	0.00000
H	2.47459	–2.24356	0.00000
C	2.92772	–4.25033	0.00000
O	2.57749	–5.41492	0.00000
C	4.37720	–3.83490	0.00000
H	4.59676	–3.22403	0.87794
H	4.59676	–3.22403	–0.87794
H	4.99924	–4.72724	0.00000
N	–1.82958	–0.74275	0.00000
H	–1.19977	0.05802	0.00000
C	–3.17604	–0.38098	0.00000
O	–3.46428	0.82008	0.00000
N	–4.10445	–1.34091	0.00000
H	–3.77415	–2.30155	0.00000
C	–5.51512	–1.01063	0.00000
H	–5.78461	–0.43145	0.88605
H	–5.78461	–0.43145	–0.88605
H	–6.08124	–1.94087	0.00000
H	1.19977	–0.05801	0.00000
N	1.82957	0.74276	0.00000
C	1.25040	1.99762	0.00000
N	–0.08561	2.01135	0.00000
C	–0.67625	3.21504	0.00000
C	0.07357	4.40204	0.00000
C	1.43797	4.25174	0.00000

N	2.04799	3.06317	0.00000
H	2.08821	5.12055	0.00000
H	–0.40285	5.36702	0.00000
C	3.17603	0.38099	0.00000
O	3.46428	–0.82008	0.00000
N	4.10444	1.34092	0.00000
H	3.77415	2.30155	0.00000
C	5.51511	1.01064	0.00000
H	5.78460	0.43145	0.88605
H	5.78460	0.43145	–0.88605
H	6.08124	1.94088	0.00000
N	–2.05121	3.18213	0.00000
H	–2.47457	2.24355	0.00000
C	–2.92772	4.25033	0.00000
O	–2.57748	5.41491	0.00000
C	–4.37720	3.83490	0.00000
H	–4.59676	3.22403	0.87794
H	–4.59676	3.22403	–0.87794
H	–4.99924	4.72724	0.00000

Sum of electronic and thermal free energy: –1471.144453 a.u.
$N_{Im} = 1$ (13.60*i* cm^{-1})

57

	X	Y	Z
N	2.40504	–0.00011	0.00000
C	1.24446	0.63377	0.00000
C	0.01507	–0.02349	0.00000
C	0.06219	–1.40509	0.00000
N	1.23076	–2.06890	0.00000
C	2.34072	–1.33617	0.00000
N	3.56634	–1.96249	0.00000
C	3.92653	–3.31959	0.00000
O	5.11729	–3.60564	0.00000
N	2.92920	–4.21698	0.00000
C	3.20936	–5.63760	0.00000
H	2.26050	–6.17249	0.00000
H	3.77889	–5.92845	0.88589
H	3.77889	–5.92845	–0.88589
H	1.97986	–3.85807	0.00000
H	4.36224	–1.34260	0.00000
C	–1.19132	–2.22762	0.00000
H	–0.91561	0.52608	0.00000
O	1.26650	1.96800	0.00000
H	2.18820	2.25227	0.00000
H	–0.94923	–3.28944	0.00000
H	–1.79534	–1.99909	0.88140

H	–1.79534	–1.99909	–0.88140

Sum of electronic and thermal free energy: –642.120436 a.u.
N_{Im} = 1 (120.38*i* cm^{-1})

57•57

	X	Y	Z
N	6.01722	–1.31273	0.00000
C	7.06886	–2.13358	0.00000
C	8.38409	–1.65101	0.00000
C	8.55230	–0.28469	0.00000
N	7.49661	0.55163	0.00000
C	6.29013	–0.00168	0.00000
N	5.17609	0.81331	0.00000
C	5.07742	2.19669	0.00000
O	3.94869	2.71199	0.00000
N	6.19533	2.92437	0.00000
C	6.15023	4.37269	0.00000
H	7.17407	4.74356	0.00000
H	5.63602	4.75090	0.88617
H	5.63602	4.75090	–0.88617
H	7.07245	2.41035	0.00000
H	4.26592	0.34362	0.00000
C	9.91642	0.33845	0.00000
H	9.21903	–2.33762	0.00000
O	6.87629	–3.43324	0.00000
H	5.90981	–3.68290	0.00000
O	4.45709	–4.37228	0.00000
C	3.32871	–3.85649	0.00000
N	3.23027	–2.47307	0.00000
N	2.21003	–4.58317	0.00000
C	2.11504	–1.65974	0.00000
N	0.91087	–2.21008	0.00000
C	–0.14657	–1.37125	0.00000
C	0.02165	–0.00785	0.00000
C	1.34114	0.47399	0.00000
N	2.39020	–0.34630	0.00000
O	1.53144	1.77314	0.00000
C	2.25377	–6.03153	0.00000
H	1.22956	–6.40141	0.00000
H	2.76766	–6.41025	0.88615
H	2.76766	–6.41025	–0.88615
H	1.33328	–4.06836	0.00000
H	4.14018	–2.00307	0.00000
C	–1.49791	–2.01521	0.00000
H	–0.81034	0.68170	0.00000
H	2.49807	2.02444	0.00000

H	–2.29623	–1.27319	0.00000
H	–1.60367	–2.65243	–0.88149
H	–1.60367	–2.65243	0.88149
H	9.83919	1.42494	0.00000
H	10.47908	0.02139	0.88137
H	10.47908	0.02139	–0.88137

Sum of electronic and thermal free energy: –1284.261646 a.u.
N_{Im} = 2 (113.29*i* cm^{-1}, 2.10*i* cm^{-1})

58

	X	Y	Z
N	0.03109	–1.33791	0.00000
C	–1.15914	–1.93355	0.00000
N	–2.34193	–1.30321	0.00000
C	–2.24870	0.02549	0.00000
N	–1.14174	0.73887	0.00000
C	–0.00948	–0.00180	0.00000
H	–3.18676	0.57340	0.00000
N	1.15455	0.66027	0.00000
H	2.02191	0.15235	0.00000
N	–1.12428	–3.30069	0.00000
H	–0.19865	–3.70359	0.00000
C	–2.14640	–4.27110	0.00000
O	–1.82098	–5.44990	0.00000
N	–3.41119	–3.82798	0.00000
H	–3.55751	–2.82436	0.00000
C	–4.52251	–4.75729	0.00000
H	–4.50278	–5.39590	–0.88610
H	–4.50278	–5.39590	0.88610
H	–5.44723	–4.18194	0.00000
H	1.15527	1.66533	0.00000

Sum of electronic and thermal free energy: –599.014128 a.u.
N_{Im} = 0

58•58

	X	Y	Z
N	1.76631	0.63825	0.00000
C	2.18612	–0.62649	0.00000
N	3.46876	–1.01338	0.00000
C	4.34653	–0.01076	0.00000
N	4.07242	1.27258	0.00000
C	2.74647	1.56304	0.00000
H	5.39620	–0.29186	0.00000
N	2.40756	2.84737	0.00000
H	1.42627	3.13778	0.00000
N	1.20310	–1.58069	0.00000
H	0.23912	–1.23551	0.00000

C	1.30412	–2.97768	0.00000
O	0.26602	–3.64227	0.00000
N	2.51931	–3.53152	0.00000
H	3.31598	–2.90178	0.00000
C	2.68023	–4.97164	0.00000
H	2.22440	–5.41899	0.88609
H	2.22440	–5.41899	–0.88609
H	3.74645	–5.19359	0.00000
H	–0.23913	1.23550	0.00000
N	–1.20312	1.58069	0.00000
C	–2.18613	0.62648	0.00000
N	–1.76632	–0.63825	0.00000
C	–2.74648	–1.56305	0.00000
N	–4.07243	–1.27258	0.00000
C	–4.34654	0.01075	0.00000
N	–3.46877	1.01338	0.00000
H	–5.39621	0.29186	0.00000
C	–1.30413	2.97767	0.00000
O	–0.26602	3.64225	0.00000
N	–2.51931	3.53153	0.00000
H	–3.31599	2.90180	0.00000
C	–2.68022	4.97165	0.00000
H	–2.22438	5.41899	0.88609
H	–2.22438	5.41899	–0.88609
H	–3.74644	5.19361	0.00000
N	–2.40756	–2.84737	0.00000
H	–1.42626	–3.13775	0.00000
H	3.14582	3.53023	0.00000
H	–3.14580	–3.53025	0.00000

Sum of electronic and thermal free energy: –1198.034552 a.u.
N_{Im} = 1 (15.24*i* cm^{-1})

59

	X	Y	Z
H	–1.94649	–2.60402	0.00000
N	–2.87023	–3.01685	0.00000
C	–2.85953	–4.39584	0.00000
N	–1.63898	–4.92474	0.00000
C	–1.60809	–6.26247	0.00000
N	–2.70035	–7.05704	0.00000
C	–3.84256	–6.39755	0.00000
N	–4.00648	–5.07572	0.00000
H	–4.75057	–6.99435	0.00000
C	–3.89315	–2.07384	0.00000
O	–3.57079	–0.90201	0.00000
C	–5.32560	–2.51822	0.00000

N	–0.40971	–6.86097	0.00000
H	0.42908	–6.30724	0.00000
H	–0.35471	–7.86451	0.00000
H	–5.94900	–1.62620	0.00000
H	–5.53738	–3.13378	–0.87469
H	–5.53738	–3.13378	0.87469

Sum of electronic and thermal free energy: –543.657349 a.u.
N_{Im} = 1 (83.55*i* cm^{-1})

59•59

	X	Y	Z
N	0.78278	1.72875	0.00000
C	1.99679	1.18168	0.00000
N	3.15176	1.84428	0.00000
C	3.01618	3.16910	0.00000
N	1.88998	3.84701	0.00000
C	0.77510	3.07805	0.00000
H	3.93683	3.74673	0.00000
N	–0.39628	3.70676	0.00000
H	–1.27419	3.18730	0.00000
N	2.01216	–0.20110	0.00000
H	1.09002	–0.64755	0.00000
C	3.07269	–1.08638	0.00000
O	2.81771	–2.28289	0.00000
C	4.49565	–0.61443	0.00000
H	–1.09002	0.64753	0.00000
N	–2.01217	0.20108	0.00000
C	–1.99680	–1.18170	0.00000
N	–0.78278	–1.72877	0.00000
C	–0.77510	–3.07807	0.00000
N	–1.88998	–3.84702	0.00000
C	–3.01619	–3.16912	0.00000
N	–3.15176	–1.84430	0.00000
H	–3.93683	–3.74675	0.00000
C	–3.07269	1.08637	0.00000
O	–2.81771	2.28288	0.00000
C	–4.49566	0.61443	0.00000
N	0.39627	–3.70677	0.00000
H	1.27418	–3.18731	0.00000
H	–0.39439	4.71237	0.00000
H	0.39439	–4.71238	0.00000
H	5.12918	–1.49926	0.00000
H	4.69819	0.00458	–0.87368
H	4.69819	0.00458	0.87368
H	–5.12918	1.49926	0.00000
H	–4.69820	–0.00459	–0.87368

H	–4.69820	–0.00459	0.87368

Sum of electronic and thermal free energy: –1087.320540 a.u.
$N_{Im} = 0$

Table S12. Gas-phase optimized structures at ωB97X-D/6-31+G(d) for monomers with a nonplanar minimum.

1

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	1.224247	2.001185	0.000000	N	–0.842274	–0.091698	0.046917
C	–0.085833	1.431106	0.000000	C	–1.737378	1.015732	–0.060066
C	2.409965	1.315101	0.000000	C	–1.190020	–1.412571	0.133771
O	–1.051234	2.170024	0.000000	O	–1.284216	2.140905	–0.133431
C	0.009090	–0.003073	0.000000	C	–3.095610	0.540825	–0.069755
N	–0.979166	–0.965307	0.000000	N	–4.283701	1.233301	–0.165495
C	1.269337	–0.584595	0.000000	C	–3.322322	–0.825176	0.012934
N	1.037443	–1.929268	0.000000	N	–4.679076	–0.962531	–0.031809
N	2.489821	0.008843	0.000000	N	–2.424375	–1.838309	0.128956
N	3.552837	2.050951	0.000000	N	–0.158123	–2.318885	0.176526
C	–0.332563	–2.096166	0.000000	H	0.691291	–2.042946	0.649212
H	–0.784169	–3.078660	0.000000	C	–5.202256	0.309103	–0.139765
H	1.219371	3.013808	0.000000	H	–6.268358	0.481185	–0.194689
H	1.745292	–2.648088	0.000000	H	0.134445	0.169264	–0.016235
H	4.429895	1.555525	0.000000	H	–0.461742	–3.257901	0.396301
H	3.560317	3.056614	0.000000	H	–5.184216	–1.835079	0.005569
Sum of electronic and ZPE corrections:							
	–542.280152				–542.280099		
Sum of electronic and thermal free energy:							
	–542.312968				–542.313048		
N_{Im} in C_s optimized structure = 1 (341i cm^{-1})							

2

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	2.465927	–1.355452	0.000000	C	3.919738	1.905407	0.220878
C	1.183457	–2.011683	0.000000	C	2.511140	1.614612	0.144629
N	0.031197	–1.375877	0.000000	N	2.009409	0.398523	0.146065
C	–0.000158	–0.007891	0.000000	C	2.838471	–0.688339	0.217413
N	1.254751	0.652893	0.000000	N	4.228439	–0.418219	0.293966
C	2.439757	–0.000986	0.000000	C	4.744352	0.833015	0.295138
N	1.138675	–3.365455	0.000000	N	1.632368	2.643691	0.043492
O	–1.010357	0.673626	0.000000	O	2.475682	–1.851523	0.222880
H	3.335781	0.610470	0.000000	H	5.824166	0.916720	0.356068
H	3.398569	–1.905337	0.000000	H	4.303791	2.917601	0.211650
H	1.209373	1.662486	0.000000	H	0.648306	2.423823	0.090552
H	0.235158	–3.814352	0.000000	H	1.919983	3.596423	0.194874
H	1.970700	–3.930972	0.000000	H	4.822875	–1.233763	0.348126
Sum of electronic and ZPE corrections:							
	–394.717877				–394.717521		
Sum of electronic and thermal free energy:							
	–394.748249				–394.748435		
N_{Im} in C_s optimized structure = 1 (119i cm^{-1})							

3

	C_s				C_1		
	X	Y	Z		X	Y	Z
O	2.513711	–2.501222	0.000000	O	–2.927997	2.034383	0.078018
C	2.763896	–1.305855	0.000000	C	–2.963904	0.813981	0.050597
C	4.138494	–0.788149	0.000000	C	–4.224982	0.063612	–0.013761
C	4.382254	0.538357	0.000000	C	–4.231481	–1.284803	–0.040840
N	3.305205	1.405945	0.000000	N	–3.019426	–1.950077	–0.008755
C	2.045351	0.900218	0.000000	C	–1.868998	–1.231573	0.049503
N	1.733304	–0.353395	0.000000	N	–1.782484	0.056979	0.079103

N	0.986730	1.806230	0.000000	N	–0.668155	–1.938042	0.078479
C	1.058233	3.191017	0.000000	C	–0.494846	–3.313485	0.059371
O	2.125436	3.804319	0.000000	O	–1.437254	–4.104146	0.027654
N	–0.140606	3.824296	0.000000	N	0.798729	–3.723718	0.093064
H	–0.998129	3.294874	0.000000	H	1.542059	–3.051165	–0.015641
H	0.093417	1.331120	0.000000	H	0.126141	–1.315038	0.147657
H	3.404932	2.420498	0.000000	H	–2.939758	–2.966313	–0.016354
C	5.734109	1.181942	0.000000	C	–5.448213	–2.155072	–0.103375
H	4.949757	–1.506360	0.000000	H	–5.149288	0.628469	–0.037502
C	–0.208177	5.275082	0.000000	C	1.124729	–5.136458	0.005655
H	6.516878	0.421088	0.000000	H	0.552327	–5.694860	0.748979
H	5.864079	1.814154	–0.885868	H	0.898810	–5.541897	–0.986182
H	5.864079	1.814154	0.885868	H	2.189506	–5.256471	0.212574
H	–1.259211	5.568089	0.000000	H	–6.351912	–1.543155	–0.125538
H	0.279604	5.686385	0.888047	H	–5.431712	–2.783188	–1.001426
H	0.279604	5.686385	–0.888047	H	–5.498341	–2.817073	0.768740
Sum of electronic and ZPE corrections:							
	–641.901723				–641.901446		
Sum of electronic and thermal free energy:							
	–641.940904				–641.941607		
N_{Im} in C_s optimized structure = 1 (65i cm^{-1})							

4

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	0.009108	–0.002513	0.000000	N	0.008568	–0.005011	–0.070327
C	–1.139702	–0.652568	0.000000	C	–1.138602	–0.653655	–0.056343
C	–1.246762	–2.078503	0.000000	C	–1.245868	–2.077661	–0.019437
C	–0.091342	–2.805083	0.000000	C	–0.091573	–2.806042	0.004959
C	1.158983	–2.142496	0.000000	C	1.158983	–2.143529	–0.014580
C	1.158944	–0.718669	0.000000	C	1.158944	–0.721535	–0.056926
N	2.308739	–0.002448	0.000000	N	2.309280	–0.004946	–0.070327
C	3.457586	–0.652439	0.000000	C	3.456486	–0.653527	–0.056343
C	3.564725	–2.078369	0.000000	C	3.563831	–2.077526	–0.019437
C	2.409346	–2.805013	0.000000	C	2.409577	–2.805973	0.004959
H	–2.221204	–2.557622	0.000000	H	–2.221149	–2.554847	–0.021756
H	–0.121615	–3.892633	0.000000	H	–0.122237	–3.893075	0.034220
H	2.439680	–3.892562	0.000000	H	2.440302	–3.893003	0.034220
H	4.539194	–2.557433	0.000000	H	4.539139	–2.554658	–0.021756
N	4.591914	0.107801	0.000000	N	4.601604	0.109116	–0.126912
H	4.496948	1.111027	0.000000	H	4.463775	1.093547	0.056831
N	–2.274073	0.107609	0.000000	N	–2.283763	0.108923	–0.126912
H	–2.179163	1.110841	0.000000	H	–2.145989	1.093362	0.056831
H	–3.192605	–0.300996	0.000000	H	–3.136727	–0.281510	0.244517
H	5.510469	–0.300753	0.000000	H	5.454590	–0.281270	0.244517
Sum of electronic and ZPE corrections:							
	–528.382185				–528.381605		
Sum of electronic and thermal free energy:							
	–528.415316				–528.415683		
N_{Im} in C_s optimized structure = 2 (318i cm^{-1}, 313i cm^{-1})							

8

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	1.261289	2.048106	0.000000	N	–0.980051	–0.836267	0.039768
C	0.043023	1.388981	0.000000	C	–2.156460	–0.093680	0.053248
C	2.480011	1.389823	0.000000	C	–0.989757	–2.227409	0.053606
N	–1.042400	2.195572	0.000000	N	–1.939190	1.255286	0.111881
C	–0.000152	0.015919	0.000000	C	–3.376195	–0.710092	0.044786
C	1.262279	–0.820966	0.000000	C	–3.505295	–2.217036	0.112473
C	2.524133	0.016791	0.000000	C	–2.166953	–2.921618	0.045158
N	3.564877	2.197162	0.000000	N	0.263154	–2.772473	0.112557

C	–1.284781	–0.630010	0.000000	H	0.987798	–2.284914	–0.397208
C	3.809208	–0.628250	0.000000	H	–1.137580	1.602099	–0.397848
O	–1.202482	–1.981370	0.000000	H	–2.790353	1.805301	0.010243
O	–2.394382	–0.087471	0.000000	H	0.266868	–3.785899	0.011171
H	–2.116114	–2.305480	0.000000	H	–0.192213	–0.405408	0.507377
O	3.727842	–1.979666	0.000000	C	–4.569646	0.102723	–0.038926
O	4.918433	–0.084944	0.000000	C	–2.126720	–4.365032	–0.038178
H	4.641698	–2.303146	0.000000	O	–5.705859	–0.629792	–0.067982
H	1.260940	3.056036	0.000000	O	–4.631985	1.331646	–0.080555
H	4.473013	1.738891	0.000000	H	–6.436358	0.005855	–0.119041
H	3.493462	3.200536	0.000000	O	–3.356583	–4.926274	–0.067248
H	–1.950220	1.736674	0.000000	O	–1.125754	–5.080735	–0.079492
H	–0.971677	3.198996	0.000000	H	–3.215670	–5.884317	–0.118042
H	1.262511	–1.488052	0.871395	H	–4.040015	–2.509262	1.026455
H	1.262511	–1.488052	–0.871395	H	–4.138442	–2.563374	–0.712204
Sum of electronic and ZPE corrections:							
		–736.974693				–736.975738	
Sum of electronic and thermal free energy:							
		–737.011997				–737.014614	
N_{Im} in C_s optimized structure = 2 (381i cm^{-1}, 305i cm^{-1})							

11

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–0.721558	–1.183380	0.000000	N	–0.760624	–1.182222	–0.014432
H	–1.729198	–1.153487	0.000000	H	–1.684821	–1.154804	–0.424837
C	–0.010836	0.001628	0.000000	C	–0.042867	–0.001105	–0.008138
C	–0.082334	–2.408437	0.000000	C	–0.114146	–2.403811	–0.008138
C	1.274907	–2.473205	0.000000	C	1.238149	–2.473909	0.033024
N	–0.916613	–3.500261	0.000000	N	–0.988019	–3.488798	–0.107053
C	1.347858	–0.014175	0.000000	C	1.311206	–0.011295	0.033024
N	–0.778923	1.140989	0.000000	N	–0.850885	1.133777	–0.107052
H	–0.518366	–4.423691	0.000000	H	–0.506287	–4.378884	–0.111272
H	–1.919126	–3.426129	0.000000	H	–1.724644	–3.489298	0.590396
H	–0.326635	2.039187	0.000000	H	–0.317235	1.993741	–0.111274
H	–1.784068	1.126417	0.000000	H	–1.586182	1.177945	0.590399
H	1.778954	–3.433319	0.000000	H	1.742153	–3.432777	0.088109
C	2.091768	–1.266842	0.000000	C	2.060508	–1.265914	0.022486
H	1.907935	0.914369	0.000000	H	1.871165	0.916010	0.088109
O	3.327546	–1.303503	0.000000	O	3.292969	–1.302477	0.043550
Sum of electronic and ZPE corrections:							
		–433.962607				–433.967308	
Sum of electronic and thermal free energy:							
		–433.994707				–433.999554	
N_{Im} in C_s optimized structure = 3 (492i cm^{-1}, 487i cm^{-1}, 130i cm^{-1})							

15

	C_s				C_1		
	X	Y	Z		X	Y	Z
C	0.052411	1.337386	0.000000	C	0.045825	1.300143	0.083332
N	0.052877	0.000055	0.000000	N	0.061186	–0.035675	0.038085
C	1.245301	–0.580465	0.000000	C	1.259587	–0.601978	–0.015311
O	1.224811	–1.919922	0.000000	O	1.254679	–1.940760	–0.062201
N	2.444780	0.000115	0.000000	N	2.451562	–0.006479	–0.024243
C	2.418712	1.340945	0.000000	C	2.410659	1.332840	0.025030
C	1.254412	2.078193	0.000000	C	1.237723	2.054799	0.079749
N	–1.163618	1.937784	0.000000	N	–1.181606	1.889688	0.101170
H	3.387814	1.834183	0.000000	H	3.373805	1.837429	0.018766
H	1.263657	3.162343	0.000000	H	1.233711	3.138416	0.110192
H	–1.989309	1.359185	0.000000	H	–1.975441	1.287794	0.264271
H	–1.261977	2.938906	0.000000	H	2.182102	–2.219198	–0.096327
H	2.149600	–2.209239	0.000000	H	–1.271192	2.857231	0.366697

Sum of electronic and ZPE corrections:							
	–394.715004				–394.714512		
Sum of electronic and thermal free energy:							
	–394.745104				–394.744887		
N_{Im} in C_s optimized structure = 1 (187i cm^{-1})							

20

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	2.948660	–0.813904	0.000000	N	2.939458	–0.803379	–0.057499
C	3.793144	0.311279	0.000000	C	3.785926	0.315119	–0.020440
C	3.347469	–2.119124	0.000000	C	3.335568	–2.109989	–0.057109
O	3.280899	1.429282	0.000000	O	3.288777	1.438914	–0.025333
C	5.207479	0.009644	0.000000	C	5.202915	0.004152	0.006970
C	5.598384	–1.302246	0.000000	C	5.590363	–1.306159	–0.004401
C	4.693510	–2.393207	0.000000	C	4.673634	–2.392524	–0.024976
N	2.360382	–3.067503	0.000000	N	2.315933	–3.049759	–0.152839
H	1.964354	–0.574906	0.000000	H	1.958261	–0.573117	–0.162022
C	6.155366	1.173185	0.000000	C	6.152979	1.164856	0.033973
H	6.663032	–1.528238	0.000000	H	6.653512	–1.537561	0.013692
H	5.045147	–3.418015	0.000000	H	5.018857	–3.419571	–0.007733
H	7.194750	0.829749	0.000000	H	7.191442	0.819978	0.056076
H	5.996980	1.808952	0.878387	H	5.973327	1.796589	0.910998
H	5.996980	1.808952	–0.878387	H	6.014039	1.804484	–0.844740
H	1.383249	–2.828808	0.000000	H	1.504724	–2.867005	0.425860
H	2.603125	–4.043465	0.000000	H	2.633195	–4.003397	–0.040478
Sum of electronic and ZPE corrections:							
	–417.935672				–417.936240		
Sum of electronic and thermal free energy:							
	–417.968205				–417.968798		
N_{Im} in C_s optimized structure = 1 (423i cm^{-1})							

22

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	2.976562	0.698649	0.000000	N	–0.846288	–0.197913	0.161302
C	3.179973	2.113841	0.000000	C	–1.693042	0.952925	0.152089
C	3.950942	–0.263997	0.000000	C	–1.248715	–1.504584	0.104190
O	2.210276	2.847806	0.000000	O	–1.190825	2.058367	0.211931
C	4.587449	2.401179	0.000000	C	–3.068668	0.540176	0.078119
N	5.257654	3.604272	0.000000	N	–4.226716	1.283412	0.053234
C	5.482159	1.338992	0.000000	C	–3.354444	–0.817497	0.036826
N	6.723921	1.903775	0.000000	N	–4.714706	–0.907102	–0.016071
N	5.231617	0.003791	0.000000	N	–2.498530	–1.874515	0.032763
N	3.542115	–1.561146	0.000000	N	–0.259251	–2.456786	0.179265
H	4.251237	–2.276424	0.000000	H	–0.591352	–3.389662	–0.025116
H	2.574030	–1.833419	0.000000	H	0.631836	–2.240466	–0.245611
C	6.517619	3.268091	0.000000	C	–5.177480	0.391769	–0.002875
C	7.984750	1.191946	0.000000	C	–5.488460	–2.130010	–0.073338
H	7.351733	3.958135	0.000000	H	–5.287044	–2.745851	0.806624
H	1.998531	0.436248	0.000000	H	–6.237966	0.606401	–0.036913
H	8.797005	1.921313	0.000000	H	0.134222	0.022186	0.288431
H	8.063430	0.562088	0.889679	H	–6.548570	–1.870938	–0.098848
H	8.063430	0.562088	–0.889679	H	–5.232452	–2.697733	–0.971400
Sum of electronic and ZPE corrections:							
	–581.553900				–581.553723		
Sum of electronic and thermal free energy:							
	–581.590100				–581.589340		
N_{Im} in C_s optimized structure = 1 (352i cm^{-1})							

26

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–0.003811	0.005342	0.000000	N	–0.129960	–0.709176	–0.123971
C	–0.009573	–1.346524	0.000000	C	–1.285330	–1.393457	0.027818
C	1.200670	0.744540	0.000000	C	1.056567	–1.339481	–0.561845
N	–1.196233	–1.988425	0.000000	N	–2.390523	–0.715129	0.421097
N	1.103565	–2.050622	0.000000	N	–1.373659	–2.681689	–0.223880
C	2.239399	–1.300694	0.000000	C	–0.211845	–3.249170	–0.652944
N	2.365458	–0.005265	0.000000	N	0.951903	–2.695289	–0.829467
N	1.094869	2.014725	0.000000	N	2.092608	–0.605317	–0.669021
H	3.161110	–1.878946	0.000000	H	–2.316084	0.182628	0.873951
H	2.027376	2.423639	0.000000	H	–0.282776	–4.313088	–0.869420
H	–0.852856	0.556586	0.000000	H	2.870264	–1.176555	–0.994204
H	–1.179297	–2.996534	0.000000	H	–0.062853	0.289114	0.030511
H	–2.082194	–1.510392	0.000000	H	–3.192901	–1.283240	0.650596
Sum of electronic and ZPE corrections:							
	–390.875549				–390.875036		
Sum of electronic and thermal free energy:							
	–390.906086				–390.905855		
N_{Im} in C_s optimized structure = 1 (189i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	2.404140	0.014186	0.000000	N	–0.849647	–0.135760	0.216693
C	2.458136	1.346690	0.000000	C	–1.774331	0.824755	0.182729
C	1.189301	–0.580463	0.000000	C	–1.255507	–1.423301	0.166356
N	3.665607	1.951210	0.000000	N	–1.378181	2.116155	0.262809
C	1.258396	2.086117	0.000000	C	–3.133972	0.468582	0.089420
N	0.989831	3.444583	0.000000	N	–4.300193	1.212390	0.026102
C	0.088946	1.334865	0.000000	C	–3.397194	–0.895961	0.052496
N	–0.917362	2.267195	0.000000	N	–4.763520	–0.979990	–0.033401
N	–0.016009	0.003882	0.000000	N	–2.506959	–1.890208	0.091748
N	1.208397	–1.940631	0.000000	N	–0.250046	–2.354611	0.157280
H	0.341234	–2.450422	0.000000	H	–0.515524	–3.300856	0.384284
H	2.089573	–2.425349	0.000000	H	–2.049701	2.849347	0.095628
H	3.730060	2.956582	0.000000	C	–5.242703	0.314265	–0.046219
H	4.501915	1.389649	0.000000	H	–6.301821	0.523687	–0.111189
C	–0.312415	3.508143	0.000000	H	–0.395031	2.323557	0.180816
H	–0.893976	4.420050	0.000000	H	0.651180	–2.041726	0.484274
H	–1.906205	2.069281	0.000000	H	–5.301490	–1.831546	–0.084026
Sum of electronic and ZPE corrections:							
	–522.410440				–522.409597		
Sum of electronic and thermal free energy:							
	–522.443091				–522.442808		
N_{Im} in C_s optimized structure = 2 (286i cm^{-1}, 88i cm^{-1})							

31

	C_s				C_1		
	X	Y	Z		X	Y	Z
N	2.402717	0.017764	0.000000	N	–0.848780	–0.133239	0.217283
C	2.455905	1.350980	0.000000	C	–1.771652	0.830001	0.185488
C	1.188770	–0.578227	0.000000	C	–1.256777	–1.419770	0.164904
N	3.663941	1.955132	0.000000	N	–1.370823	2.120599	0.270094
C	1.256335	2.089591	0.000000	C	–3.131543	0.477665	0.091680
N	0.981346	3.445027	0.000000	N	–4.297809	1.218174	0.028429
C	0.087629	1.337341	0.000000	C	–3.397599	–0.886303	0.052351
N	–0.930110	2.255725	0.000000	N	–4.761972	–0.983989	–0.035602
N	–0.016941	0.004776	0.000000	N	–2.508907	–1.883954	0.090011
N	1.209776	–1.939124	0.000000	N	–0.251811	–2.353473	0.153094
H	0.343325	–2.449973	0.000000	H	–0.520195	–3.297538	0.386099

H	2.091601	–2.422590	0.000000	H	–2.039649	2.854046	0.092829
H	3.728097	2.960505	0.000000	C	–5.234745	0.311978	–0.045699
H	4.500174	1.393540	0.000000	C	–5.522485	–2.213246	–0.104398
C	–0.323144	3.495120	0.000000	H	–6.296227	0.515433	–0.111723
C	–2.345186	1.954287	0.000000	H	–6.581855	–1.967026	–0.201295
H	–0.913492	4.402826	0.000000	H	–0.387757	2.323563	0.175823
H	–2.905012	2.891820	0.000000	H	0.647601	–2.041542	0.486347
H	–2.607405	1.374886	–0.889077	H	–5.205876	–2.802449	–0.968768
H	–2.607405	1.374886	0.889077	H	–5.368619	–2.804661	0.802012
Sum of electronic and ZPE corrections:							
		–561.684068				–561.683205	
Sum of electronic and thermal free energy:							
		–561.719925				–561.719220	
N_{Im} in C_s optimized structure = 2 (293i cm^{-1}, 116i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	0.886747	0.048495	0.000000	N	0.886126	0.046207	0.078210
C	1.483681	1.230339	0.000000	C	1.482050	1.228426	0.043771
C	2.880760	1.325141	0.000000	C	2.878616	1.322249	0.004917
C	3.540880	0.092428	0.000000	C	3.538358	0.089498	0.013204
N	2.991811	–1.122689	0.000000	N	2.987989	–1.124776	0.049507
C	1.656838	–1.066285	0.000000	C	1.654723	–1.067894	0.074232
N	0.983725	–2.246027	0.000000	N	0.976862	–2.255106	0.061312
O	0.720497	2.323223	0.000000	O	0.719196	2.321156	0.049110
N	3.782615	2.376701	0.000000	N	3.780236	2.372852	–0.034116
C	4.945671	1.793741	0.000000	C	4.942960	1.788943	–0.049402
N	4.871136	0.413462	0.000000	N	4.868359	0.409362	–0.021475
H	5.637191	–0.242500	0.000000	H	5.634089	–0.247001	–0.030986
H	5.898787	2.305320	0.000000	H	5.895850	2.299970	–0.080689
H	–0.202105	2.022889	0.000000	H	–0.203382	2.021477	0.072197
H	1.497107	–3.111376	0.000000	H	1.504159	–3.080617	0.301146
H	–0.022091	–2.248179	0.000000	H	0.007060	–2.230067	0.335692
Sum of electronic and ZPE corrections:							
		–542.276864				–542.276376	
Sum of electronic and thermal free energy:							
		–542.309464				–542.309141	
N_{Im} in C_s optimized structure = 1 (262i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–0.632226	1.182478	0.000000	N	–0.643487	1.184047	–0.018641
C	–1.962802	1.182740	0.000000	C	–1.972628	1.180893	–0.015100
C	–0.014797	–0.004449	0.000000	C	–0.021886	–0.000934	–0.009094
N	–2.559983	2.407970	0.000000	N	–2.578809	2.412648	0.029849
C	–2.755788	–0.005933	0.000000	C	–2.762214	–0.007565	–0.007262
C	–2.074573	–1.199356	0.000000	C	–2.078724	–1.200880	–0.007598
C	–0.668778	–1.240484	0.000000	C	–0.673602	–1.238054	–0.007658
N	1.361047	0.026510	0.000000	N	1.353829	0.033760	–0.005733
C	2.100783	–1.122682	0.000000	C	2.096105	–1.113545	–0.000612
H	1.799559	0.936028	0.000000	H	1.790187	0.944362	–0.003083
C	–4.257966	0.073475	0.000000	C	–4.264400	0.069952	0.008592
H	–2.606745	–2.147408	0.000000	H	–2.608751	–2.150088	–0.002393
C	0.078830	–2.509636	0.000000	C	0.077988	–2.506104	–0.004248
H	–4.694578	–0.928731	0.000000	H	–4.699850	–0.931081	0.066651
H	–3.558704	2.519769	0.000000	H	3.170995	–0.967823	0.002756
H	–1.977205	3.229699	0.000000	C	1.528450	–2.343288	–0.000131
H	3.176017	–0.979424	0.000000	O	–0.480089	–3.604024	–0.004895
C	1.530070	–2.350796	0.000000	H	2.146203	–3.233497	0.003555

O	–0.481377	–3.606887	0.000000	H	–4.628021	0.643825	0.870400
H	2.145377	–3.242719	0.000000	H	–4.660799	0.544481	–0.899825
H	–4.638450	0.597039	0.887402	H	–3.528714	2.498588	–0.296999
H	–4.638450	0.597039	–0.887402	H	–1.977913	3.199118	–0.171591
Sum of electronic and ZPE corrections:							
		–587.540884				–587.540478	
Sum of electronic and thermal free energy:							
		–587.576427				–587.576197	
N_{Im} in C_s optimized structure = 1 (283i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–0.004972	0.002853	0.000000	N	–0.052463	–0.746853	0.201049
C	0.065745	–1.332789	0.000000	C	–1.076805	–1.605541	0.154792
N	1.201223	–2.060938	0.000000	N	–1.031719	–2.904479	0.515138
C	2.304484	–1.322413	0.000000	C	0.161894	–3.293796	0.946852
N	2.385455	0.002747	0.000000	N	1.260597	–2.555415	1.048350
C	1.183874	0.615703	0.000000	C	1.088773	–1.277095	0.654018
N	1.187077	1.965223	0.000000	N	2.168514	–0.468754	0.714723
N	–1.097786	–2.016462	0.000000	N	–2.264315	–1.133369	–0.280883
H	3.248132	–1.863919	0.000000	H	2.071497	0.509601	0.497028
H	2.065416	2.457563	0.000000	H	–2.329067	–0.189619	–0.626028
H	0.315373	2.469000	0.000000	H	0.249486	–4.334533	1.251603
H	–1.079691	–3.023215	0.000000	H	3.023640	–0.820558	1.113698
H	–1.972560	–1.518035	0.000000	H	–3.036172	–1.770930	–0.390152
Sum of electronic and ZPE corrections:							
		–390.908373				–390.907999	
Sum of electronic and thermal free energy:							
		–390.939648				–390.939730	
N_{Im} in C_s optimized structure = 1 (67i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	0.009108	–0.002513	0.000000	N	0.008568	–0.005011	–0.070327
C	–1.139702	–0.652568	0.000000	C	–1.138602	–0.653655	–0.056343
C	–1.246762	–2.078503	0.000000	C	–1.245868	–2.077661	–0.019437
C	–0.091342	–2.805083	0.000000	C	–0.091573	–2.806042	0.004959
C	1.158983	–2.142496	0.000000	C	1.158983	–2.143529	–0.014580
C	1.158944	–0.718669	0.000000	C	1.158944	–0.721535	–0.056926
N	2.308739	–0.002448	0.000000	N	2.309280	–0.004946	–0.070327
C	3.457586	–0.652439	0.000000	C	3.456486	–0.653527	–0.056343
C	3.564725	–2.078369	0.000000	C	3.563831	–2.077526	–0.019437
C	2.409346	–2.805013	0.000000	C	2.409577	–2.805973	0.004959
H	–2.221204	–2.557622	0.000000	H	–2.221149	–2.554847	–0.021756
H	–0.121615	–3.892633	0.000000	H	–0.122237	–3.893075	0.034220
H	2.439680	–3.892562	0.000000	H	2.440302	–3.893003	0.034220
H	4.539194	–2.557433	0.000000	H	4.539139	–2.554658	–0.021756
N	4.591914	0.107801	0.000000	N	4.601604	0.109116	–0.126912
H	4.496948	1.111027	0.000000	H	4.463775	1.093547	0.056831
N	–2.274073	0.107609	0.000000	N	–2.283763	0.108923	–0.126912
H	–2.179163	1.110841	0.000000	H	–2.145989	1.093362	0.056831
H	–3.192605	–0.300996	0.000000	H	–3.136727	–0.281510	0.244517
H	5.510469	–0.300753	0.000000	H	5.454590	–0.281270	0.244517
Sum of electronic and ZPE corrections:							
		–563.353831				–563.353289	
Sum of electronic and thermal free energy:							
		–563.389086				–563.388725	
N_{Im} in C_s optimized structure = 1 (230i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
O	2.206696	4.024250	0.000000	O	3.277924	1.638225	0.026901
C	2.175672	2.809068	0.000000	C	3.027068	0.449203	0.032601
N	3.414121	2.101619	0.000000	N	4.118465	–0.470263	0.061551
C	3.516869	0.764282	0.000000	C	3.978896	–1.803263	0.062332
C	2.384839	–0.000668	0.000000	C	2.726983	–2.351777	0.041926
C	1.161943	0.732430	0.000000	C	1.654868	–1.410419	0.023404
N	1.042785	2.038486	0.000000	N	1.774210	–0.104440	0.015397
N	–0.003951	0.007131	0.000000	N	0.378620	–1.915845	0.003861
C	–0.029323	–1.373225	0.000000	C	0.108574	–3.269220	–0.012001
C	1.124784	–2.110818	0.000000	C	1.105998	–4.200972	0.008066
N	–1.274631	–1.923791	0.000000	N	–1.232364	–3.574465	–0.101404
H	–0.855981	0.552870	0.000000	H	–1.873353	–2.969658	0.395825
C	2.421628	–1.482812	0.000000	H	–0.362082	–1.237763	–0.123323
H	4.505624	0.316156	0.000000	C	2.498747	–3.815039	0.027157
H	4.238105	2.689737	0.000000	H	4.870831	–2.421948	0.076720
O	3.493095	–2.090036	0.000000	H	5.034714	–0.039774	0.075006
H	1.077425	–3.193581	0.000000	O	3.439658	–4.607700	0.043706
H	–1.376632	–2.925073	0.000000	H	0.866268	–5.257911	0.019993
H	–2.114618	–1.369476	0.000000	H	–1.453943	–4.552962	0.019024
Sum of electronic and ZPE corrections:							
	–639.516563				–639.516518		
Sum of electronic and thermal free energy:							
	–639.552039				–639.552067		
N_{Im} in C_s optimized structure = 1 (346i cm^{-1})							

45

	C_s				C_1		
	X	Y	Z		X	Y	Z
H	0.152445	–2.334732	0.000000	H	0.151030	–2.338640	–0.036950
N	1.104265	–1.991377	0.000000	N	1.101360	–1.993410	0.006330
C	1.144757	–0.602272	0.000000	C	1.142510	–0.603880	0.000210
N	0.001479	0.000837	0.000000	N	0.000000	0.000000	0.000000
C	0.025164	1.380084	0.000000	C	0.024640	1.379400	–0.002060
C	1.235500	2.105224	0.000000	C	1.235450	2.103670	0.000000
C	2.515029	1.390017	0.000000	C	2.514450	1.387480	–0.000180
N	2.365360	0.002640	0.000000	N	2.363710	0.000000	0.000000
O	3.621060	1.899649	0.000000	O	3.620900	1.896010	–0.001750
C	1.196037	3.501933	0.000000	C	1.196810	3.500500	–0.001270
N	–1.171896	1.992076	0.000000	N	–1.172020	1.991910	–0.004660
C	2.176049	–2.872972	0.000000	C	2.171320	–2.875380	–0.001910
O	3.344271	–2.506196	0.000000	O	3.339090	–2.512790	–0.046930
N	1.820738	–4.185901	0.000000	N	1.807980	–4.192580	0.007290
H	2.567656	–4.862961	0.000000	H	2.567350	–4.846070	0.131330
H	0.869053	–4.515836	0.000000	H	0.898910	–4.490590	0.327480
H	3.199220	–0.586434	0.000000	H	3.197560	–0.588510	–0.016760
H	2.129898	4.056064	0.000000	H	2.130950	4.054170	–0.000360
C	–0.036105	4.126027	0.000000	C	–0.035050	4.125180	–0.003860
C	–1.182680	3.317667	0.000000	C	–1.182130	3.317480	–0.005590
H	–2.169004	3.777893	0.000000	H	–2.168160	3.778280	–0.007940
H	–0.127245	5.206871	0.000000	H	–0.125610	5.206070	–0.004810
Sum of electronic and ZPE corrections:							
	–732.963028				–732.962499		
Sum of electronic and thermal free energy:							
	–733.001311				–733.001070		
N_{Im} in C_s optimized structure = 1 (191i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z

N	0.001497	–0.000579	0.000000	N	–0.334518	1.756008	–0.081974
C	1.155961	0.594950	0.000000	C	0.927718	2.061422	–0.068221
N	2.370270	–0.001771	0.000000	N	1.455187	3.304175	0.021802
C	2.448399	–1.383538	0.000000	C	0.609655	4.396212	0.112103
C	1.252885	–2.108259	0.000000	C	–0.768474	4.161334	0.104395
C	–0.050325	–1.390280	0.000000	C	–1.283611	2.769180	0.003959
N	3.667906	–1.920295	0.000000	N	1.180297	5.596903	0.200738
O	–1.109887	–1.993131	0.000000	O	–2.479038	2.530926	–0.003485
N	1.115883	1.983141	0.000000	N	1.806831	0.989781	–0.161047
H	0.163504	2.325287	0.000000	H	1.313847	0.106154	–0.184279
C	2.189617	2.862978	0.000000	C	3.193476	1.027524	–0.162067
N	1.837751	4.176234	0.000000	N	3.785331	–0.198178	–0.266480
O	3.356899	2.492263	0.000000	O	3.834852	2.063727	–0.048024
H	0.886532	4.507686	0.000000	H	3.290592	–1.002213	–0.621768
H	3.213062	0.572536	0.000000	H	2.467946	3.421452	0.040757
H	2.585812	4.852058	0.000000	H	4.786446	–0.186132	–0.394419
C	1.348107	–3.499174	0.000000	C	–1.606873	5.271550	0.196030
H	0.433599	–4.084445	0.000000	H	–2.681329	5.115370	0.192424
C	2.605229	–4.084579	0.000000	C	–1.039641	6.533527	0.288950
H	2.727740	–5.162256	0.000000	H	–1.652414	7.425452	0.362251
C	3.727509	–3.250380	0.000000	C	0.354791	6.637921	0.287220
H	4.728611	–3.674614	0.000000	H	0.833942	7.611256	0.359257
Sum of electronic and ZPE corrections:							
		–732.959521				–732.959002	
Sum of electronic and thermal free energy:							
		–732.997929				–732.997708	
N_{Im} in C_s optimized structure = 1 (176i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–3.184496	1.707199	0.000000	N	–3.191033	1.723284	–0.123549
C	–3.188898	0.338546	0.000000	C	–3.189718	0.341695	–0.054855
C	–4.390303	–0.392503	0.000000	C	–4.386388	–0.392183	–0.076535
C	–4.298332	–1.773482	0.000000	C	–4.291799	–1.773679	–0.049507
C	–3.059736	–2.413600	0.000000	C	–3.051308	–2.407468	–0.009137
C	–1.936036	–1.588685	0.000000	C	–1.930202	–1.578902	0.002075
N	–1.990857	–0.251527	0.000000	N	–1.991334	–0.242524	–0.014196
N	–0.616010	–2.054663	0.000000	N	–0.609058	–2.041993	0.024756
C	–0.166089	–3.360763	0.000000	C	–0.158076	–3.342698	0.114915
O	–0.892363	–4.342242	0.000000	O	–0.877604	–4.319778	0.236590
N	1.201905	–3.471800	0.000000	N	1.223466	–3.441814	0.101148
H	1.582565	–4.404292	0.000000	H	1.549518	–4.392657	–0.000576
H	1.836583	–2.690312	0.000000	H	1.761642	–2.758420	–0.412795
H	0.054235	–1.297727	0.000000	H	0.063049	–1.287299	0.065525
H	–2.958643	–3.488913	0.000000	H	–2.947358	–3.482264	0.019964
H	–5.204972	–2.372302	0.000000	H	–5.195934	–2.375978	–0.061115
H	–5.350056	0.114539	0.000000	H	–5.346314	0.112387	–0.121304
H	–4.037899	2.238287	0.000000	H	–4.013485	2.194167	0.224340
H	–2.302957	2.193181	0.000000	H	–2.320424	2.155067	0.154254
Sum of electronic and ZPE corrections:							
		–527.423004				–527.422743	
Sum of electronic and thermal free energy:							
		–527.458302				–527.458269	
N_{Im} in C_s optimized structure = 2 (361i cm^{-1} ,321i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
O	1.063457	2.023390	0.000000	O	1.069622	1.997093	–0.302107
C	1.119592	0.809186	0.000000	C	1.120170	0.791106	–0.159597
N	2.390003	0.184022	0.000000	N	2.387368	0.166428	–0.066804

C	2.551266	–1.154573	0.000000	C	2.543344	–1.159951	0.121778
C	1.472339	–1.981345	0.000000	C	1.460238	–1.976968	0.202719
C	0.190933	–1.337901	0.000000	C	0.183393	–1.337835	0.073176
N	0.037395	–0.033714	0.000000	N	0.033349	–0.043772	–0.085776
N	–1.016421	–2.017406	0.000000	N	–1.021287	–2.018434	0.150678
C	–1.422662	–3.349621	0.000000	C	–1.413838	–3.352513	0.077196
O	–2.617155	–3.576192	0.000000	O	–2.597249	–3.604152	0.196332
H	1.614207	–3.048475	0.000000	H	1.590060	–3.029697	0.390383
H	3.570930	–1.524314	0.000000	H	3.560689	–1.524927	0.212132
H	3.182989	0.811931	0.000000	H	3.182808	0.788398	–0.126484
H	–1.805773	–1.377048	0.000000	H	–1.814596	–1.384384	0.187175
C	–0.406263	–4.464417	0.000000	C	–0.394507	–4.437865	–0.169626
H	–0.957889	–5.404636	0.000000	H	–0.944846	–5.346321	–0.415729
H	0.228171	–4.424123	–0.890865	H	0.284427	–4.187934	–0.989593
H	0.228171	–4.424123	0.890865	H	0.194165	–4.627652	0.734148
Sum of electronic and ZPE corrections:							
		–547.285723				–547.285733	
Sum of electronic and thermal free energy:							
		–547.319924				–547.321980	
N_{Im} in C_s optimized structure = 1 (24i cm^{-1})							

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	C_s				C_1		
	X	Y	Z		X	Y	Z
N	–3.267555	–1.760828	0.000000	N	–3.291119	–1.766308	–0.112610
C	–3.140729	–0.403112	0.000000	C	–3.148101	–0.404062	–0.007443
C	–4.284600	0.433529	0.000000	C	–4.281219	0.433527	0.132958
C	–4.094594	1.795356	0.000000	C	–4.083592	1.793462	0.181554
C	–2.797208	2.328370	0.000000	C	–2.787030	2.321396	0.090945
C	–1.751978	1.403715	0.000000	C	–1.749590	1.394969	–0.037677
N	–1.895489	0.074475	0.000000	N	–1.904991	0.067565	–0.085371
N	–0.448565	1.859861	0.000000	N	–0.448853	1.847668	–0.127034
C	–0.144108	3.197568	0.000000	C	–0.142768	3.184531	–0.113934
C	–1.133351	4.144357	0.000000	C	–1.115857	4.131539	0.016771
N	1.190577	3.497163	0.000000	N	1.205832	3.463796	–0.292943
H	1.905737	2.789967	0.000000	H	1.841362	2.878266	0.235903
H	0.270867	1.150475	0.000000	H	0.251946	1.162278	–0.374551
C	–2.531515	3.783833	0.000000	C	–2.516284	3.774470	0.118129
H	–4.931315	2.487883	0.000000	H	–4.912826	2.487404	0.283595
H	–5.279673	–0.000299	0.000000	H	–5.275959	0.002540	0.187415
O	–3.451714	4.606750	0.000000	O	–3.423553	4.601148	0.234150
H	–0.876205	5.197734	0.000000	H	–0.853137	5.182757	0.059585
H	1.483562	4.459418	0.000000	H	1.433139	4.442821	–0.180791
H	–2.437432	–2.330970	0.000000	H	–2.447661	–2.306850	0.015282
H	–4.168523	–2.207273	0.000000	H	–4.133548	–2.184951	0.251057
Sum of electronic and ZPE corrections:							
		–603.589468				–603.589805	
Sum of electronic and thermal free energy:							
		–603.624932				–603.625432	
N_{Im} in C_s optimized structure = 2 (418i cm^{-1}, 300i cm^{-1})							