

Anion Recognition using Enhanced Halogen Bonding through Intramolecular Hydrogen Bonds – A Computational Insight

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Supplementary Material

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Table S1. Analysis of the bond situation between the receptors (**1d–h** and **2d–m**) and anions (Cl⁻) through the EDA–NOCV methodology. The energy unit is kcal mol⁻¹.^[a,b]

Complex	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}	$\Delta E_{\text{oi},1}$	$\Delta E_{\text{oi},2}$
1d ...Cl ⁻	-37.78	-46.64 (48)	59.77	-48.51 (50)	-2.39 (2)	-37.46	-
1e ...Cl ⁻	-22.75	-28.14 (45)	39.31	-31.62 (51)	-2.30 (4)	-23.16	-
1f ...Cl ⁻	-40.33	-48.52 (53)	51.93	-41.37 (45)	-2.37 (3)	-31.13	-
1g ...Cl ⁻	-20.92	-25.97 (44)	37.57	-30.23 (52)	-2.28 (4)	-22.15	-
1h ...Cl ⁻	-32.38	-39.22 (50)	45.38	-36.21 (47)	-2.33 (3)	-25.76	-
2d ...Cl ⁻	-156.01	-167.99 (72)	77.89	-60.57 (26)	-5.35 (2)	-32.14	-13.63
2e ...Cl ⁻	-165.72	-179.11 (71)	87.96	-69.08 (27)	-5.48 (2)	-37.58	-15.42
2f ...Cl ⁻	-148.82	-161.15 (71)	79.63	-62.05 (27)	-5.25 (2)	-32.88	-14.35
2g ...Cl ⁻	-166.34	-178.52 (72)	83.05	-65.57 (26)	-5.30 (2)	-33.97	-14.30
2h ...Cl ⁻	-151.63	-164.29 (71)	80.60	-62.72 (27)	-5.22 (2)	-32.75	-14.52
2i ...Cl ⁻	-165.80	-177.25 (72)	81.20	-64.30 (26)	-5.45 (2)	-34.66	-13.89
2j ...Cl ⁻	-150.68	-163.35 (71)	79.73	-61.78 (27)	-5.28 (2)	-32.65	-13.97
2k ...Cl ⁻	-163.04	-176.88 (71)	84.85	-65.85 (27)	-5.15 (2)	-34.08	-15.78
2l ...Cl ⁻	-154.13	-166.87 (71)	80.70	-62.70 (27)	-5.25 (2)	-33.01	-14.42
2m ...Cl ⁻	-161.85	-174.71 (72)	82.06	-63.91 (26)	-5.29 (2)	-33.92	-14.31

^[a] $\Delta E_{\text{int}} = \Delta V_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}}$; ^[b] Values in parentheses correspond to the percentage of each stabilizing contribution: $\Delta V_{\text{elstat}} (\%) + \Delta E_{\text{oi}} (\%) + \Delta E_{\text{disp}} (\%) = 100\%$.

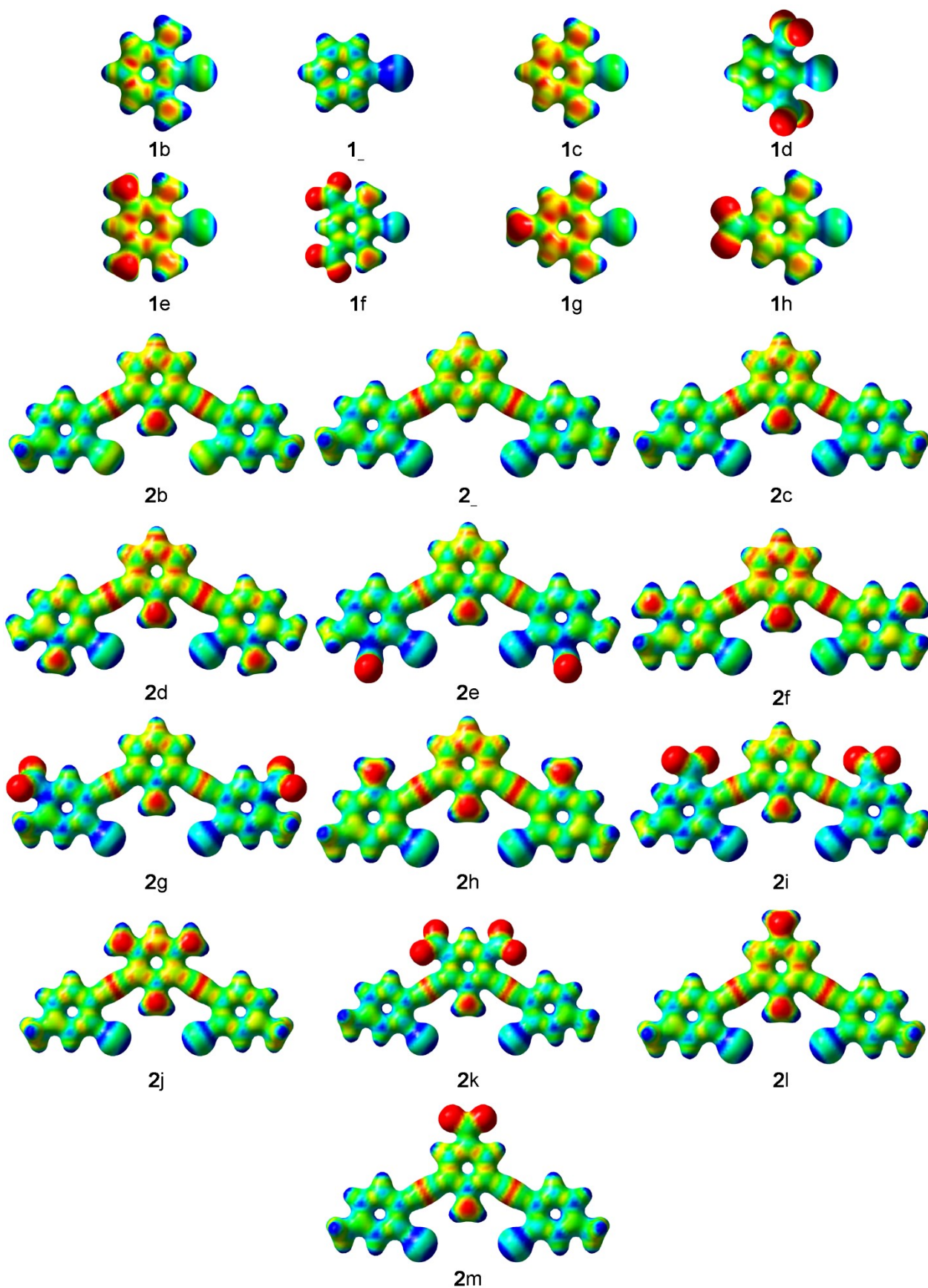


Figure S1. Electrostatic potential surfaces mapped to an electronic density of 0.050 a.u.: i) [0.100 a.u. (red) to 0.250 a.u. (blue)] for 1₋ or b receptor; ii) [0.100 a.u. (red) to 0.350 a.u. (blue)] for 1(c–h) receptors; and iii) [0.300 a.u. (red) to 0.500 a.u. (blue)] for 2₋ or b–m receptors.

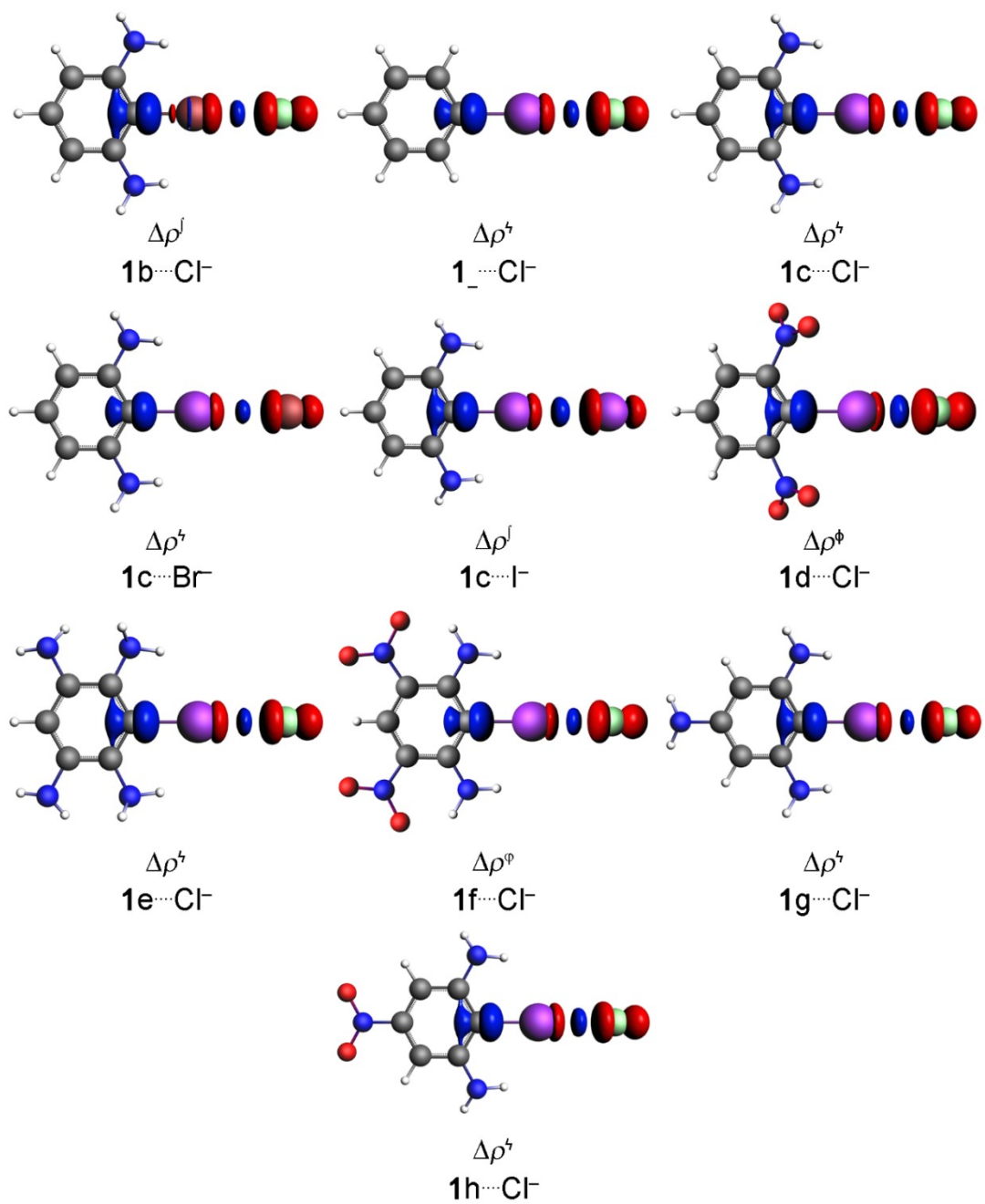


Figure S2. The first density deformation channel surface plots, $\Delta\rho_1$, with isovalues = $\int 0.003$, \int = and $\phi 0.005$ a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, for the **1**(₋ or b-h)...(Cl⁻, Br⁻ or I⁻) complexes. Color code for atoms: H = white; C = gray; N = blue; Cl = green; Br = wine; and I = purple.

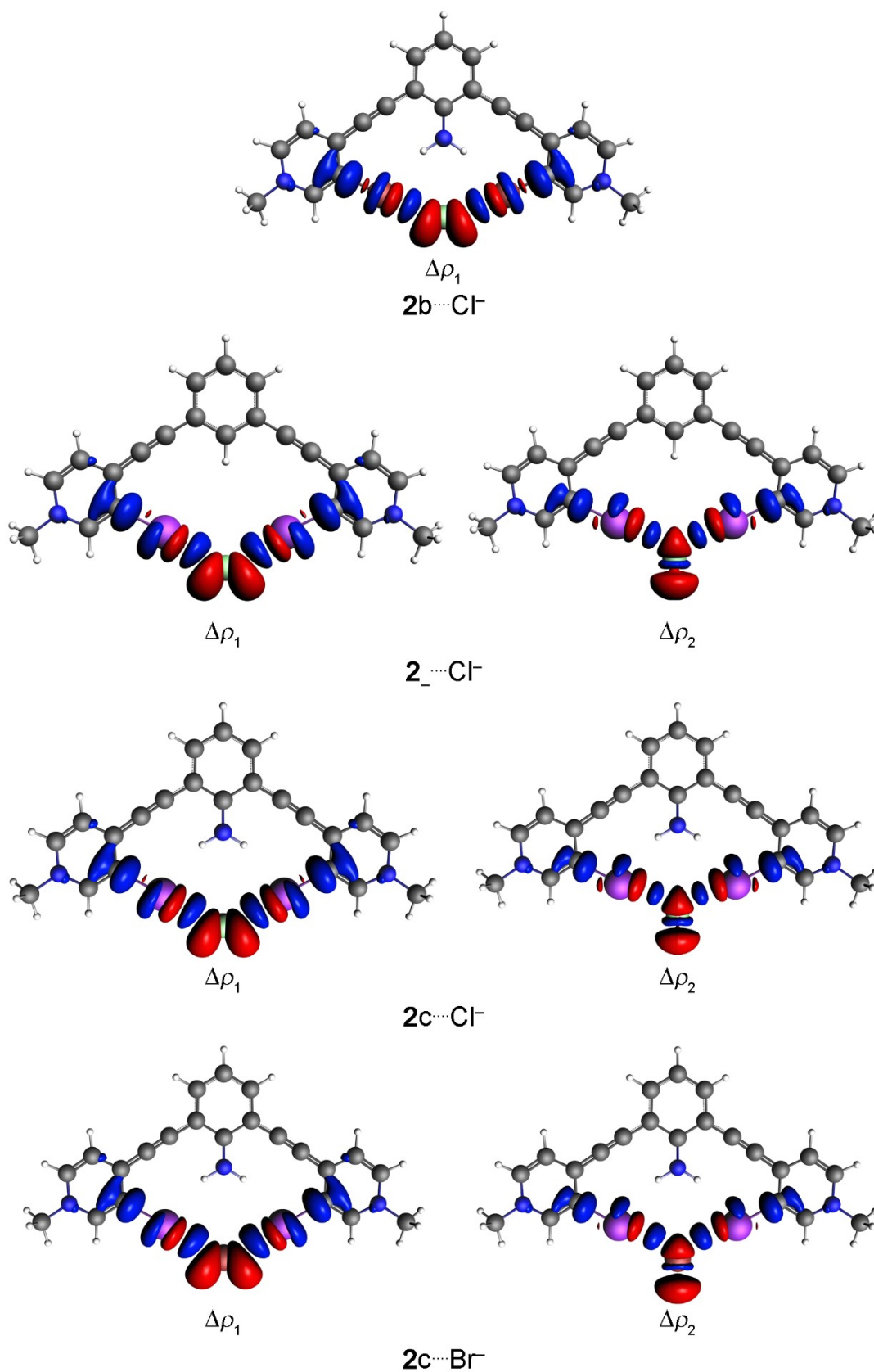


Figure S3. The first two density deformation channel surface plots, $\Delta\rho_{1,2}$, with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, for the $2(-, b \text{ or } c) \cdots (Cl^- \text{ or } Br^-)$ complexes. Color code for atoms: H = white; C = gray; N = blue; Cl = green; and Br = wine.

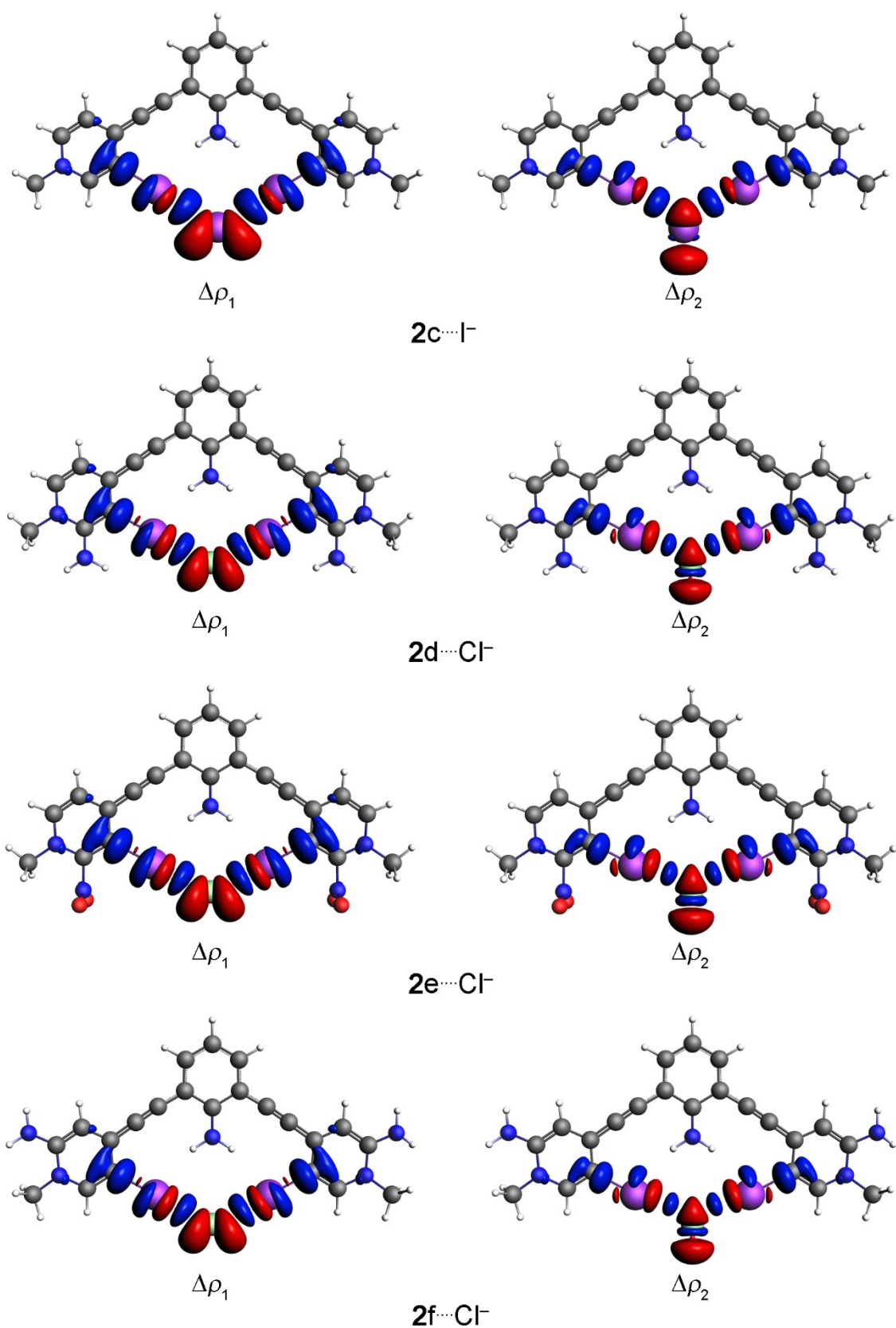


Figure S4. The first two density deformation channel surface plots, $\Delta\rho_{1,2}$, with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, for the **2c**...I⁻ and **2(d-f)**...Cl⁻ complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; and I = purple.

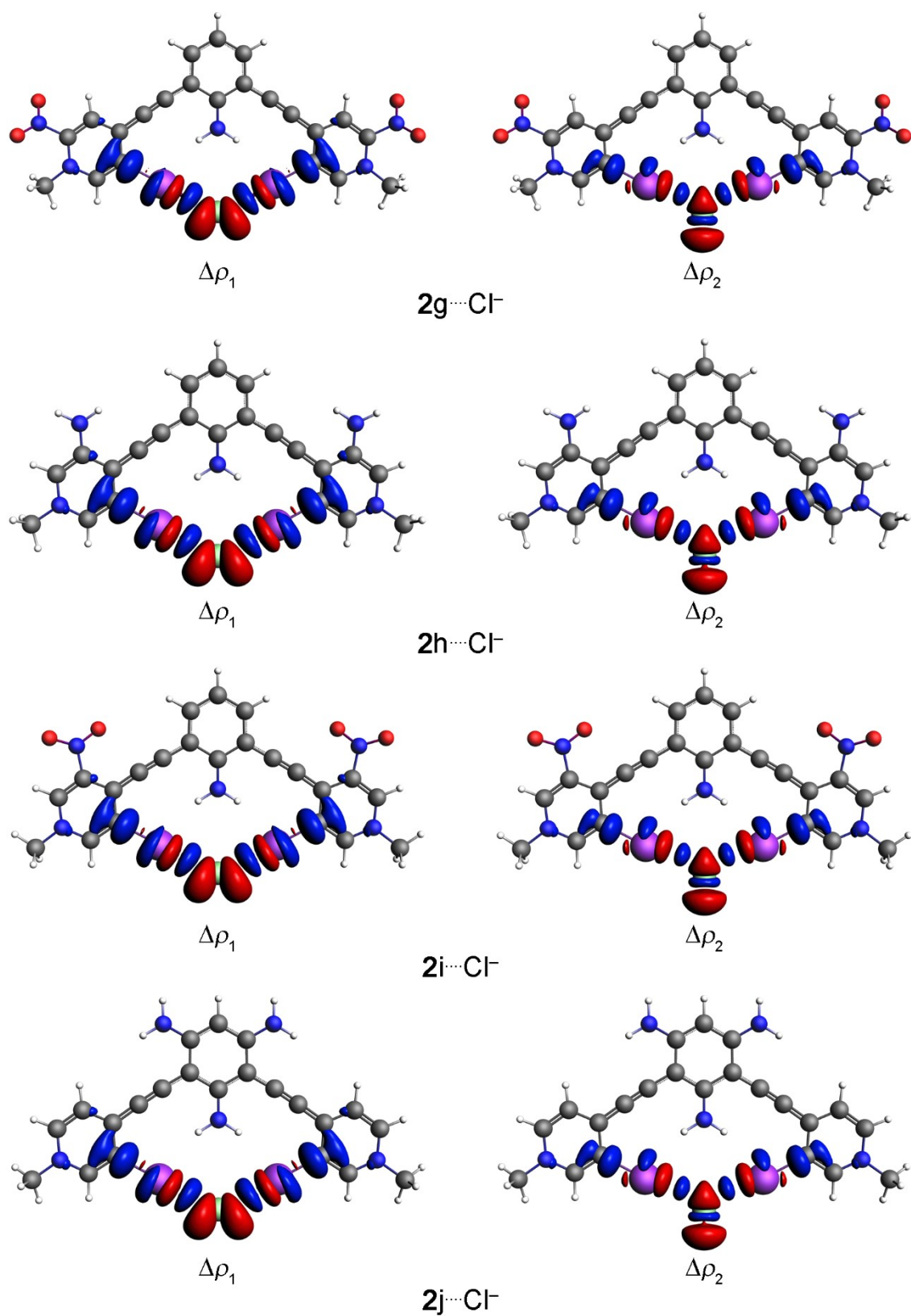


Figure S5. The first two density deformation channel surface plots, $\Delta\rho_{1,2}$, with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, for the **2(g-j)···Cl⁻** complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; and I = purple.

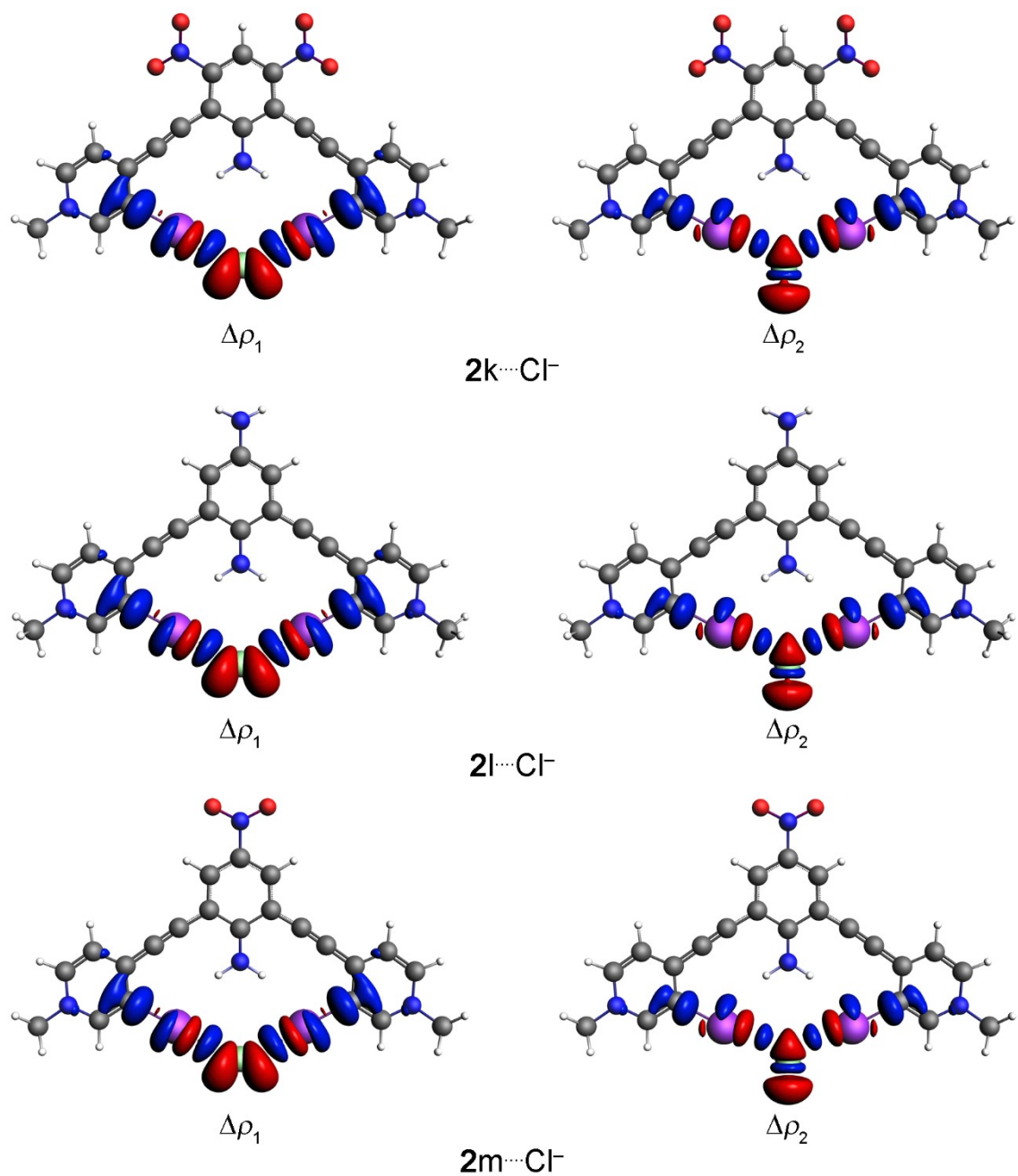


Figure S6. The first two density deformation channel surface plots, $\Delta\rho_{1,2}$, with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, for the **2(l and m)...**Cl⁻ complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; and I = purple.

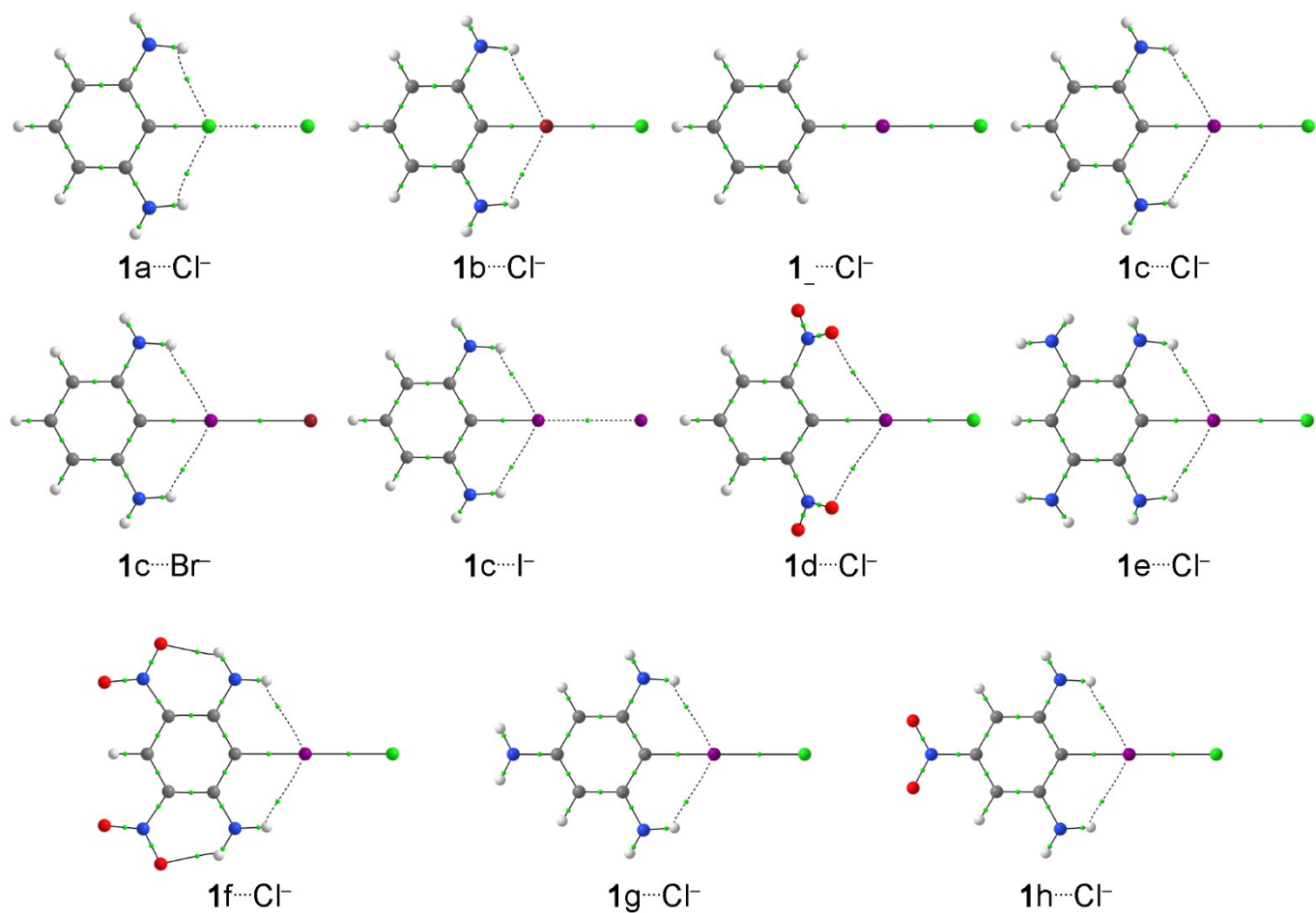


Figure S7. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the 1(_ or a-h)...(Cl⁻, Br⁻ or I⁻) complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; Br = brown; and I = purple.

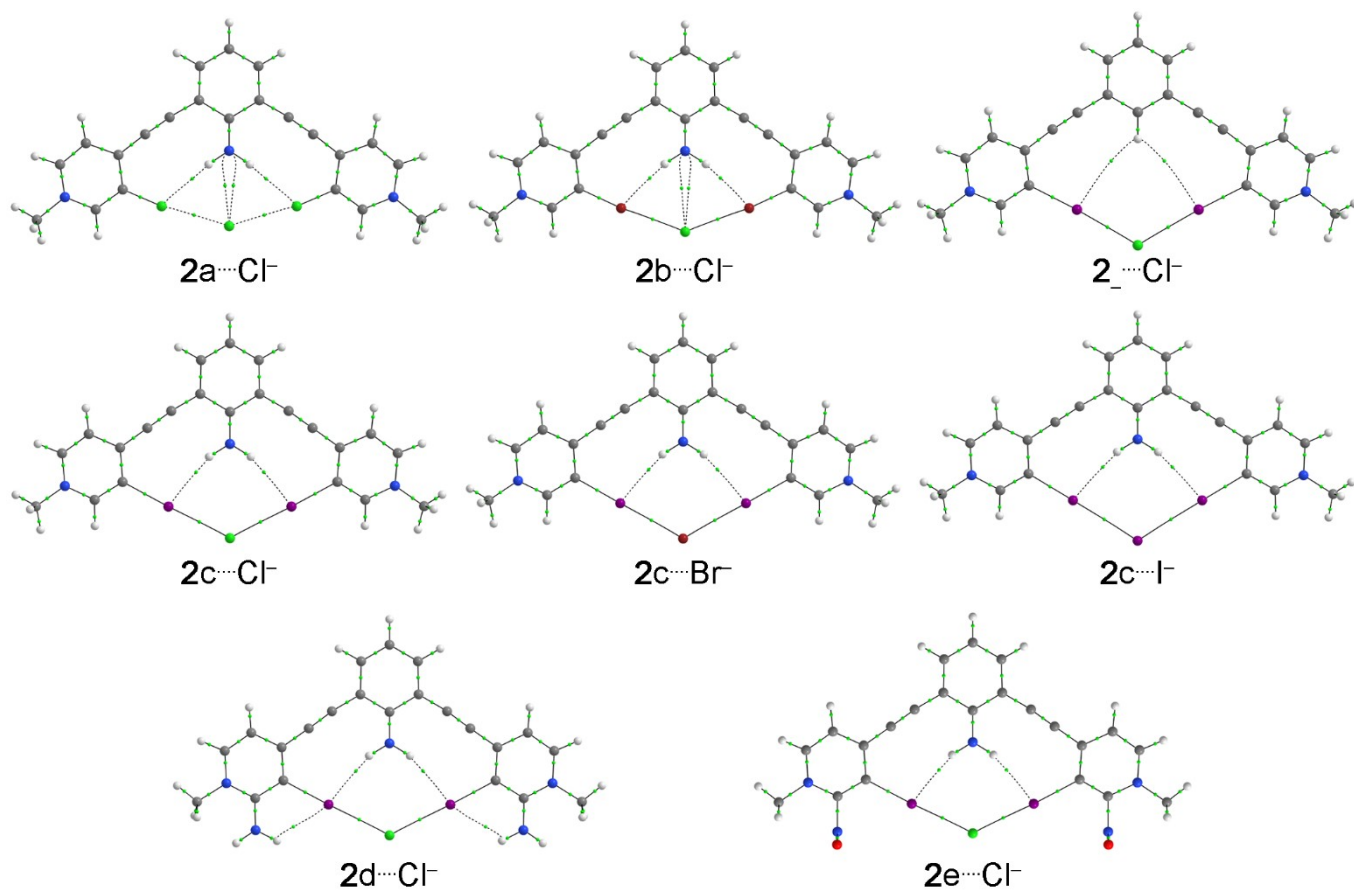


Figure S8. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the **2**(₋ or a-e)⋯(Cl⁻, Br⁻ or I⁻) complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; Br = brown; and I = purple.

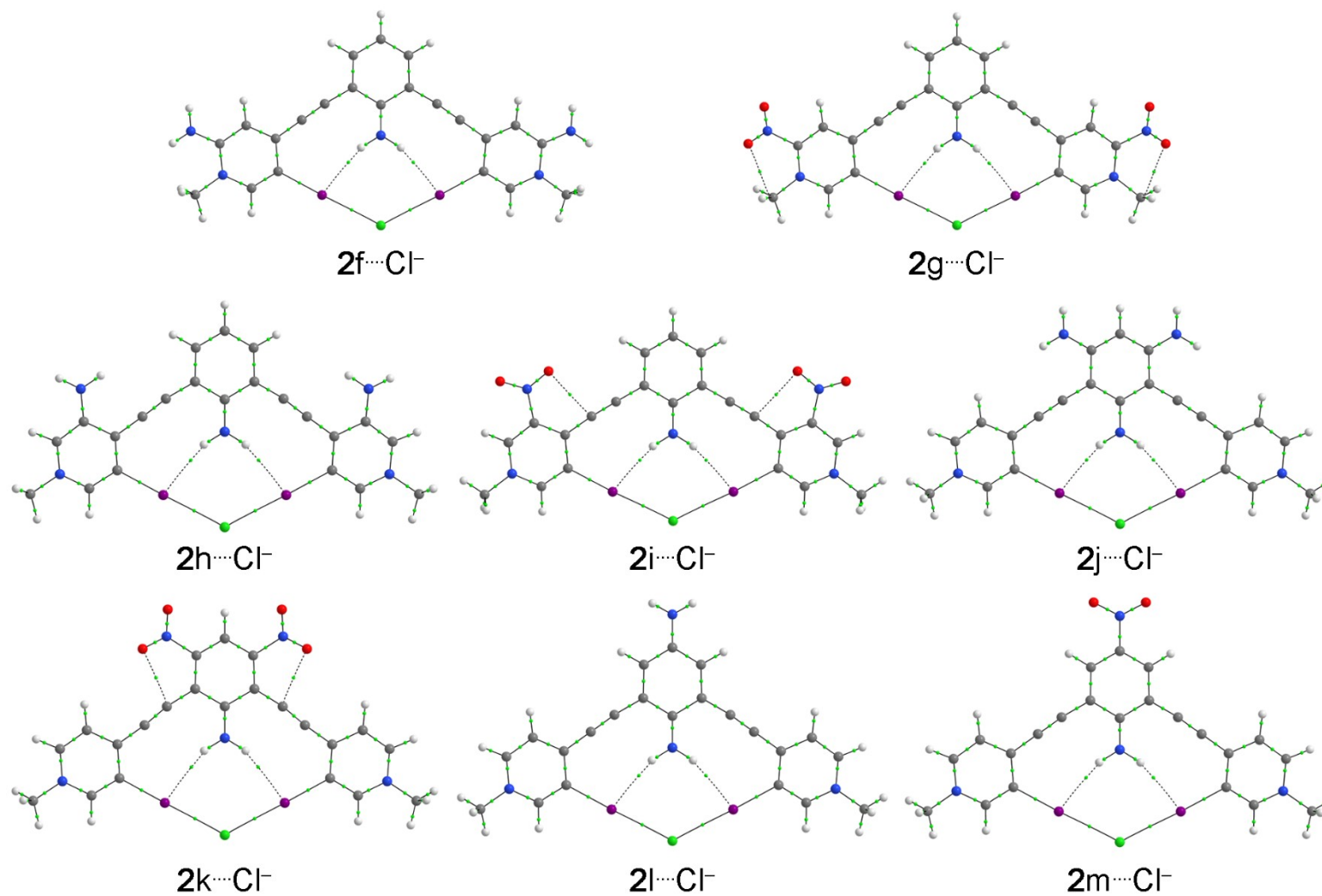


Figure S9. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the $2(f-m)\cdots\text{Cl}^-$ complexes. Color code for atoms: H = white; C = gray; N = blue; O = red; Cl = green; and I = purple.

Table S2. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to the interactions present in **1**($_$ or a-h) \cdots (Cl $^-$, Br $^-$ or I $^-$) complexes. The values of all parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
1a \cdots Cl $^-$	C-Cl \cdots Cl $^-$	1.106	0.022
	N-H \cdots Cl	1.229	0.017
	N-H \cdots Cl	1.229	0.017
1b \cdots Cl $^-$	C-Br \cdots Cl $^-$	1.014	0.028
	N-H \cdots Br	1.185	0.016
	N-H \cdots Br	1.185	0.016
1c \cdots Br $^-$	C-I \cdots Br $^-$	0.941	0.027
	N-H \cdots I	1.172	0.015
	N-H \cdots I	1.172	0.015
1 $_$ \cdots Cl $^-$	C-I \cdots Cl $^-$	0.916	0.033
	C-I \cdots Cl $^-$	0.916	0.033
	N-H \cdots I	1.169	0.015
1c \cdots Cl $^-$	N-H \cdots I	1.169	0.015
	C-I \cdots I $^-$	0.964	0.021
	N-H \cdots I	1.175	0.015
1c \cdots I $^-$	N-H \cdots I	1.175	0.015
	C-I \cdots Cl $^-$	0.805	0.046
	N-O \cdots I	1.293	0.010
1d \cdots Cl $^-$	N-O \cdots I	1.293	0.010
	C-I \cdots Cl $^-$	0.911	0.034
	N-H \cdots I	1.154	0.016
1e \cdots Cl $^-$	N-H \cdots I	1.154	0.016
	C-I \cdots Cl $^-$	0.845	0.041
	N-H \cdots I	1.155	0.016
1f \cdots Cl $^-$	N-H \cdots I	1.155	0.016
	C-I \cdots Cl $^-$	0.921	0.032
	N-H \cdots I	1.169	0.015
1g \cdots Cl $^-$	N-H \cdots I	1.169	0.015
	C-I \cdots Cl $^-$	0.879	0.037
	N-H \cdots I	1.173	0.015
1h \cdots Cl $^-$	N-H \cdots I	1.173	0.015
	C-I \cdots Cl $^-$	0.879	0.037
	N-H \cdots I	1.173	0.015

Table S3. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to the interactions present in **2**(- or a-c)···(Cl⁻, Br⁻ or I⁻) complexes. The values of all parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
2a ···Cl ⁻	C–Cl···Cl ⁻	1.094	0.023
	C–Cl···Cl ⁻	1.094	0.023
	N–H···Cl	1.472	0.009
	N–H···Cl	1.472	0.009
	N···Cl ⁻	1.246	0.013
	N···Cl ⁻	1.246	0.013
2b ···Cl ⁻	C–Br···Cl ⁻	0.994	0.030
	C–Br···Cl ⁻	0.994	0.030
	N–H···Br	1.309	0.012
	N–H···Br	1.309	0.012
	N···Br ⁻	1.352	0.007
	N···Br ⁻	1.352	0.007
2c ···Br ⁻	C–I···Br ⁻	0.901	0.031
	C–I···Br ⁻	0.901	0.031
	N–H···I	1.229	0.014
	N–H···I	1.229	0.014
2 ···Cl ⁻	C–I···Cl ⁻	0.890	0.036
	C–I···Cl ⁻	0.890	0.036
	C–H···I	1.537	0.002
	C–H···I	1.537	0.002
2c ···Cl ⁻	C–I···Cl ⁻	0.907	0.034
	C–I···Cl ⁻	0.907	0.034
	N–H···I	1.208	0.015
	N–H···I	1.208	0.015
2c ···I ⁻	C–I···I ⁻	0.885	0.028
	C–I···I ⁻	0.885	0.028
	N–H···I	1.251	0.012
	N–H···I	1.251	0.012

Table S4. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to the interactions present in **2**(d–m)···Cl⁻ complexes. The values of all parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
2d ···Cl ⁻	C–I···Cl ⁻	0.917	0.033
	C–I···Cl ⁻	0.917	0.033
	N–H···I	1.241	0.014
	N–H···I	1.241	0.014
	N–H···I	1.173	0.016
	N–H···I	1.173	0.016
2e ···Cl ⁻	C–I···Cl ⁻	0.886	0.036
	C–I···Cl ⁻	0.886	0.036
	N–H···I	1.204	0.015
	N–H···I	1.204	0.015
2f ···Cl ⁻	C–I···Cl ⁻	0.911	0.034
	C–I···Cl ⁻	0.910	0.034
	N–H···I	1.207	0.015
	N–H···I	1.207	0.015
2g ···Cl ⁻	C–I···Cl ⁻	0.901	0.035
	C–I···Cl ⁻	0.901	0.035
	N–H···I	1.210	0.015
	N–H···I	1.210	0.015
2h ···Cl ⁻	C–I···Cl ⁻	0.908	0.034
	C–I···Cl ⁻	0.908	0.034
	N–H···I	1.214	0.014
	N–H···I	1.214	0.014
2i ···Cl ⁻	C–I···Cl ⁻	0.907	0.034
	C–I···Cl ⁻	0.907	0.034
	N–H···I	1.174	0.017
	N–H···I	1.173	0.017
2j ···Cl ⁻	C–I···Cl ⁻	0.912	0.034
	C–I···Cl ⁻	0.912	0.034
	N–H···I	1.203	0.015
	N–H···I	1.203	0.015
2k ···Cl ⁻	C–I···Cl ⁻	0.895	0.035
	C–I···Cl ⁻	0.895	0.035
	N–H···I	1.236	0.013
	N–H···I	1.236	0.013
2l ···Cl ⁻	C–I···Cl ⁻	0.908	0.034
	C–I···Cl ⁻	0.908	0.034
	N–H···I	1.206	0.015
	N–H···I	1.206	0.015
2m ···Cl ⁻	C–I···Cl ⁻	0.904	0.034
	C–I···Cl ⁻	0.904	0.034
	N–H···I	1.207	0.015
	N–H···I	1.207	0.015

Table S5. Optimized Cartesian coordinates for the compounds investigated in this study using the BLYP–D3(BJ)/Def2–TZVP computational model.

1a^{•••}Cl⁻

C	1.275086000	1.226727000	-0.037535000
C	0.583278000	-0.000042000	-0.085291000
C	2.681949000	1.216353000	0.074730000
C	1.275404000	-1.226642000	-0.037522000
C	3.367019000	0.000305000	0.136599000
C	2.682263000	-1.215917000	0.074753000
N	0.569865000	2.434192000	-0.142918000
N	0.570533000	-2.434331000	-0.142894000
H	3.223592000	2.162273000	0.103481000
H	4.453430000	0.000446000	0.226343000
H	3.224140000	-2.161700000	0.103521000
H	0.983108000	3.210203000	0.364840000
H	-0.430177000	2.335012000	0.027832000
H	0.983975000	-3.210168000	0.364977000
H	-0.429537000	-2.335412000	0.027875000
Cl	-1.207191000	-0.000278000	-0.107844000
Cl	-4.156416000	0.000020000	0.109456000

1b^{•••}Cl⁻

C	-1.566051000	-1.223645000	-0.029593000
C	-0.869345000	0.000001000	-0.066698000
C	-2.975498000	-1.214899000	0.066121000
C	-1.566125000	1.223614000	-0.029595000
C	-3.662139000	-0.000070000	0.120079000
C	-2.975563000	1.214798000	0.066133000
N	-0.874840000	-2.441981000	-0.129668000
N	-0.874963000	2.441966000	-0.129639000
H	-3.517155000	-2.161402000	0.086901000
H	-4.749678000	-0.000096000	0.197484000
H	-3.517266000	2.161274000	0.086946000
H	-1.305433000	-3.210551000	0.375833000
H	0.123279000	-2.354864000	0.059824000
H	-1.305667000	3.210602000	0.375654000
H	0.123150000	2.354938000	0.059892000
Br	1.129201000	0.000057000	-0.056807000
Cl	4.033157000	-0.000035000	0.106010000

1c...Br⁻

C	-2.401300000	-1.220963000	-0.020960000
C	-1.696293000	-0.000005000	-0.061567000
C	-3.810936000	-1.213238000	0.083325000
I	0.528599000	-0.000007000	-0.059891000
C	-2.401260000	1.220989000	-0.020912000
C	-4.498213000	0.000020000	0.141152000
C	-3.810913000	1.213256000	0.083322000
N	-1.727870000	-2.450090000	-0.128031000
N	-1.727797000	2.450052000	-0.127991000
H	-4.351862000	-2.160237000	0.106978000
H	-5.585282000	0.000040000	0.225573000
H	-4.351840000	2.160260000	0.106992000
H	-2.174582000	-3.215148000	0.369314000
H	-0.729122000	-2.386279000	0.068635000
H	-2.174635000	3.215320000	0.368883000
H	-0.729066000	2.386310000	0.068704000
Br	3.656679000	0.000000000	0.069290000

1...Cl⁻

C	-2.013761000	1.207047000	-0.000013000
C	-1.295105000	0.000168000	-0.000117000
C	-3.414913000	1.208245000	0.000138000
C	-2.013215000	-1.207037000	-0.000013000
C	-4.123704000	-0.000474000	0.000208000
C	-3.414363000	-1.208872000	0.000144000
H	-3.955205000	2.156499000	0.000213000
H	-5.213657000	-0.000721000	0.000325000
H	-3.954221000	-2.157371000	0.000213000
I	0.915732000	0.000285000	-0.000152000
Cl	3.834223000	-0.000484000	0.000312000
H	-1.471569000	2.152509000	-0.000027000
H	-1.470553000	-2.152255000	-0.000050000

1c...Cl⁻

C	-1.861238000	-1.219194000	-0.028677000
C	-1.152489000	-0.000074000	-0.063569000
C	-3.271607000	-1.212890000	0.064966000
I	1.080273000	-0.000070000	-0.037413000
C	-1.860925000	1.219287000	-0.028679000
C	-3.959917000	0.000244000	0.118100000
C	-3.271328000	1.213197000	0.064965000

N	-1.186332000	-2.449897000	-0.130288000
N	-1.185798000	2.449730000	-0.130187000
H	-3.812705000	-2.160105000	0.084175000
H	-5.047732000	0.000391000	0.194295000
H	-3.812264000	2.160515000	0.084260000
H	-1.631434000	-3.210169000	0.376325000
H	-0.188754000	-2.379590000	0.072048000
H	-1.631019000	3.210467000	0.375538000
H	-0.188209000	2.379488000	0.071952000
Cl	3.995740000	0.000029000	0.104999000

1c...I⁻

C	-2.885118000	1.222352000	0.014771000
C	-2.183569000	0.000077000	0.059617000
C	-4.294236000	1.212869000	-0.097244000
I	0.038171000	0.000505000	0.074964000
H	-4.835469000	2.159406000	-0.124190000
C	-2.884319000	-1.222824000	0.014765000
C	-4.979957000	-0.000841000	-0.158699000
H	-6.066424000	-0.001247000	-0.249107000
C	-4.293399000	-1.214126000	-0.097479000
H	-4.834101000	-2.160971000	-0.124915000
N	-2.213069000	2.450552000	0.125559000
H	-2.660744000	3.218496000	-0.365955000
H	-1.213369000	2.391663000	-0.065873000
N	-2.211526000	-2.450375000	0.125696000
H	-2.659687000	-3.219403000	-0.363618000
H	-1.212005000	-2.391553000	-0.066524000
I	3.425557000	-0.000178000	-0.052567000

1d...Cl⁻

C	1.700418000	1.174437000	0.023285000
C	0.935325000	-0.000001000	0.142156000
C	3.077346000	1.202866000	-0.218058000
I	-1.336798000	0.000002000	0.018453000
C	1.700415000	-1.174441000	0.023286000
C	3.776926000	-0.000005000	-0.328546000
C	3.077343000	-1.202874000	-0.218057000
N	1.068196000	2.522304000	0.175676000
O	0.326839000	2.707913000	1.145005000
O	1.371158000	3.388279000	-0.668109000
N	1.068188000	-2.522305000	0.175676000

O	0.326837000	-2.707914000	1.145009000
O	1.371141000	-3.388278000	-0.668114000
H	3.581578000	2.161260000	-0.314988000
H	4.851025000	-0.000007000	-0.501433000
H	3.581572000	-2.161269000	-0.314986000
Cl	-4.052532000	0.000003000	-0.381221000

1e...Cl⁻

C	-1.405400000	-1.220193000	-0.009877000
C	-0.706334000	0.000015000	-0.024797000
C	-2.817280000	-1.216601000	0.032011000
I	1.528828000	0.000012000	-0.018572000
C	-1.405431000	1.220194000	-0.009893000
C	-3.509938000	-0.000015000	0.067085000
C	-2.817306000	1.216585000	0.032008000
N	-0.758799000	-2.495957000	-0.091376000
N	-0.758797000	2.495969000	-0.091365000
N	-3.498188000	-2.470915000	0.081751000
N	-3.498230000	2.470876000	0.081736000
H	-4.602078000	-0.000029000	0.094762000
H	-0.979679000	-3.077274000	0.721021000
H	0.255542000	-2.372153000	-0.133597000
H	-0.979826000	3.077359000	0.720940000
H	0.255551000	2.372143000	-0.133339000
H	-2.986386000	-3.165630000	-0.468363000
H	-4.454472000	-2.396294000	-0.263964000
H	-4.454517000	2.396224000	-0.263963000
H	-2.986441000	3.165560000	-0.468430000
Cl	4.439566000	-0.000014000	0.046752000

1f...Cl⁻

C	0.718360000	1.231719000	0.000208000
C	0.033504000	-0.000067000	0.000282000
C	2.171996000	1.212149000	0.000048000
I	-2.228462000	-0.000116000	0.000141000
C	0.718467000	-1.231812000	0.000246000
C	2.852340000	0.000067000	-0.000047000
C	2.172121000	-1.212085000	0.000065000
N	0.030476000	2.399681000	0.000495000
N	0.030673000	-2.399830000	0.000627000
N	2.987098000	2.413267000	-0.000236000
O	2.420355000	3.545164000	-0.000494000

O	4.231853000	2.306759000	0.000057000
N	2.987460000	-2.413039000	-0.000224000
O	4.232184000	-2.306191000	0.000068000
O	2.421020000	-3.545086000	-0.000592000
H	3.934672000	0.000120000	-0.000236000
H	0.553871000	3.268912000	-0.000343000
H	-0.984514000	2.357615000	0.000006000
H	0.554139000	-3.269015000	-0.000414000
H	-0.984323000	-2.357849000	0.000012000
Cl	-5.038786000	0.000046000	-0.000484000

1g...Cl-

C	-1.535568000	-1.213913000	-0.047977000
C	-0.819909000	-0.000117000	-0.078295000
C	-2.945656000	-1.210761000	0.027544000
I	1.410915000	-0.000222000	-0.034849000
C	-1.535267000	1.213921000	-0.047968000
C	-3.646520000	0.000217000	0.070393000
C	-2.945376000	1.211017000	0.027549000
N	-0.865280000	-2.448145000	-0.139884000
N	-0.864879000	2.447995000	-0.139915000
N	-5.066566000	0.000387000	0.213129000
H	-3.488550000	-2.158163000	0.041588000
H	-3.488092000	2.158527000	0.041596000
H	-1.309772000	-3.200520000	0.379226000
H	0.132127000	-2.375141000	0.063147000
H	-1.309215000	3.200500000	0.379110000
H	0.132619000	2.374978000	0.062607000
H	-5.490886000	-0.829874000	-0.197441000
H	-5.490681000	0.830825000	-0.197297000
Cl	4.334165000	0.000400000	0.119629000

1h...Cl-

C	-0.987366000	1.223916000	0.085096000
C	-0.275085000	-0.000012000	0.101884000
C	-2.393465000	1.224088000	0.025888000
I	1.948207000	-0.000051000	0.031832000
C	-0.987396000	-1.223920000	0.085093000
C	-3.065713000	0.000016000	-0.010264000
C	-2.393491000	-1.224070000	0.025879000
N	-0.308674000	2.445538000	0.172320000
N	-0.308692000	-2.445536000	0.172281000

N	-4.532806000	0.000030000	-0.086974000
O	-5.130160000	1.099504000	-0.119379000
O	-5.130185000	-1.099431000	-0.119348000
H	-2.959567000	2.150564000	0.011765000
H	-2.959605000	-2.150537000	0.011732000
H	-0.781131000	3.231011000	-0.263926000
H	0.682136000	2.389574000	-0.059259000
H	-0.781148000	-3.231041000	-0.263899000
H	0.682131000	-2.389589000	-0.059258000
Cl	4.800665000	0.000107000	-0.167016000

1a

C	-0.306242000	-1.235794000	-0.008787000
C	0.370823000	0.000000000	-0.011667000
C	-1.716411000	-1.215992000	0.003731000
C	-0.306242000	1.235794000	-0.008787000
C	-2.399286000	0.000000000	0.011265000
C	-1.716411000	1.215992000	0.003731000
N	0.390280000	-2.441830000	-0.074266000
N	0.390281000	2.441830000	-0.074266000
H	-2.259354000	-2.159760000	-0.000084000
H	-3.487948000	0.000000000	0.022950000
H	-2.259354000	2.159760000	-0.000084000
H	-0.112663000	-3.250283000	0.275436000
H	1.359539000	-2.407301000	0.225949000
H	-0.112662000	3.250283000	0.275436000
H	1.359539000	2.407300000	0.225949000
Cl	2.146564000	0.000000000	0.004544000

1b

C	0.786973000	1.236808000	-0.008453000
C	0.111347000	0.000000000	-0.011898000
C	2.198205000	1.215257000	0.004142000
C	0.786973000	-1.236808000	-0.008453000
C	2.881068000	0.000000000	0.011320000
C	2.198205000	-1.215257000	0.004142000
N	0.102138000	2.448653000	-0.074089000
N	0.102138000	-2.448653000	-0.074089000
H	2.740751000	2.159323000	0.001031000
H	3.969733000	0.000000000	0.023168000
H	2.740751000	-2.159323000	0.001031000
H	0.616873000	3.254001000	0.265520000

H	-0.866346000	2.428470000	0.230887000
H	0.616873000	-3.254001000	0.265520000
H	-0.866346000	-2.428470000	0.230887000
Br	-1.833110000	0.000000000	0.002126000

1_l

C	-1.258498000	1.218769000	0.000202000
C	-0.572463000	-0.000010000	0.000092000
C	-2.658877000	1.210062000	0.000425000
C	-1.258505000	-1.218773000	0.000202000
C	-3.361268000	0.000004000	0.000538000
C	-2.658893000	-1.210053000	0.000426000
H	-3.196926000	2.156763000	0.000511000
H	-4.449547000	0.000014000	0.000712000
H	-3.196940000	-2.156755000	0.000511000
I	1.563832000	0.000000000	-0.000250000
H	-0.714317000	2.159516000	0.000116000
H	-0.714344000	-2.159532000	0.000116000

1_c

C	1.185123000	1.236014000	-0.006093000
C	0.503327000	0.000000000	-0.009950000
C	2.597073000	1.214009000	0.003059000
I	-1.643874000	0.000000000	0.000039000
C	1.185123000	-1.236014000	-0.006093000
C	3.280683000	0.000000000	0.007537000
C	2.597073000	-1.214009000	0.003059000
N	0.513998000	2.456078000	-0.070158000
N	0.513998000	-2.456078000	-0.070158000
H	3.139168000	2.158467000	0.000222000
H	4.369405000	0.000000000	0.016815000
H	3.139168000	-2.158467000	0.000222000
H	1.045400000	3.256814000	0.254938000
H	-0.449815000	2.454784000	0.251955000
H	1.045399000	-3.256814000	0.254938000
H	-0.449815000	-2.454784000	0.251955000

1_d

C	-1.190407000	1.142090000	-0.003713000
C	0.000000000	0.395219000	-0.000003000
C	-1.204086000	2.538288000	0.029315000
I	-0.000001000	-1.725413000	-0.000004000

C	1.190408000	1.142087000	0.003708000
C	0.000003000	3.241171000	-0.000010000
C	1.204090000	2.538284000	-0.029328000
N	-2.531460000	0.486997000	-0.052730000
O	-3.336359000	0.812518000	0.830043000
O	-2.746904000	-0.299263000	-0.980516000
N	2.531461000	0.486993000	0.052744000
O	2.746894000	-0.299263000	0.980535000
O	3.336370000	0.812509000	-0.830022000
H	-2.160468000	3.053010000	0.065759000
H	0.000004000	4.328128000	-0.000014000
H	2.160473000	3.053004000	-0.065772000

1e

C	0.749713000	1.237148000	-0.001800000
C	0.079609000	0.000000000	-0.012928000
C	2.164780000	1.220648000	0.008141000
I	-2.069682000	0.000000000	-0.003933000
C	0.749713000	-1.237148000	-0.001800000
C	2.846961000	0.000000000	0.015226000
C	2.164781000	-1.220648000	0.008141000
N	0.109715000	2.496010000	-0.051957000
N	0.109716000	-2.496010000	-0.051957000
N	2.840605000	2.471131000	0.059878000
N	2.840606000	-2.471130000	0.059878000
H	3.937923000	0.000000000	-0.001537000
H	0.540925000	3.166705000	0.585829000
H	-0.894354000	2.443052000	0.110285000
H	0.540924000	-3.166704000	0.585831000
H	-0.894353000	-2.443053000	0.110282000
H	2.466817000	3.137551000	-0.618588000
H	3.845304000	2.375387000	-0.072905000
H	3.845304000	-2.375387000	-0.072909000
H	2.466815000	-3.137552000	-0.618584000

1f

C	-0.112913000	1.251194000	-0.000005000
C	0.549284000	-0.000001000	-0.000017000
C	-1.558682000	1.212447000	0.000038000
I	2.692181000	-0.000002000	-0.000080000
C	-0.112914000	-1.251195000	0.000011000
C	-2.232449000	0.000001000	0.000066000

C	-1.558684000	-1.212447000	0.000054000
N	0.559201000	2.421504000	-0.000031000
N	0.559202000	-2.421504000	0.000000000
N	-2.381776000	2.421232000	0.000054000
O	-1.812728000	3.547208000	0.000029000
O	-3.615555000	2.298441000	0.000092000
N	-2.381783000	-2.421228000	0.000085000
O	-3.615561000	-2.298430000	0.000123000
O	-1.812743000	-3.547208000	0.000076000
H	-3.316150000	0.000001000	0.000098000
H	0.006820000	3.277825000	-0.000019000
H	1.571911000	2.426564000	-0.000061000
H	0.006823000	-3.277826000	0.000022000
H	1.571912000	-2.426561000	-0.000031000

1g

C	0.859247000	1.230402000	-0.005570000
C	0.167141000	0.000000000	-0.009475000
C	2.266465000	1.213294000	0.003147000
I	-1.976660000	0.000000000	-0.001161000
C	0.859247000	-1.230402000	-0.005570000
C	2.970033000	0.000000000	0.007206000
C	2.266465000	-1.213294000	0.003147000
N	0.191184000	2.454428000	-0.070615000
N	0.191184000	-2.454428000	-0.070615000
N	4.373394000	0.000000000	0.083222000
H	2.807698000	2.159323000	0.004824000
H	2.807698000	-2.159323000	0.004824000
H	0.718814000	3.248191000	0.277667000
H	-0.773500000	2.447165000	0.249523000
H	0.718814000	-3.248191000	0.277667000
H	-0.773500000	-2.447165000	0.249523000
H	4.817526000	0.839680000	-0.276876000
H	4.817526000	-0.839680000	-0.276876000

1h

C	0.318584000	1.239297000	-0.009007000
C	-0.364278000	0.000000000	-0.009261000
C	1.728070000	1.223940000	-0.006827000
I	-2.501905000	0.000000000	0.002570000
C	0.318584000	-1.239297000	-0.009006000
C	2.387922000	0.000000000	-0.005569000

C	1.728070000	-1.223941000	-0.006826000
N	-0.349630000	2.453877000	-0.067137000
N	-0.349630000	-2.453877000	-0.067132000
N	3.877856000	0.000000000	0.005067000
O	4.457536000	1.098474000	0.009926000
O	4.457536000	-1.098474000	0.009913000
H	2.297033000	2.148092000	-0.009626000
H	2.297034000	-2.148093000	-0.009624000
H	0.184561000	3.268421000	0.213973000
H	-1.317340000	2.463747000	0.239877000
H	0.184561000	-3.268422000	0.213973000
H	-1.317342000	-2.463747000	0.239877000

2a...Cl⁻

Cl	-2.784206000	-1.695507000	-0.010718000
Cl	2.784167000	-1.695473000	-0.010719000
Cl	0.000002000	-2.515043000	-0.031352000
N	-6.765008000	-1.321246000	0.021360000
N	6.764973000	-1.321294000	0.021392000
C	-5.494639000	-1.829170000	0.011122000
C	-4.386457000	-1.002836000	0.004663000
C	-4.562440000	0.421565000	0.010733000
C	-5.899449000	0.901957000	0.022361000
C	-6.965458000	0.029201000	0.025276000
C	-3.458224000	1.273688000	0.007588000
C	-2.451493000	1.974096000	0.004460000
C	-1.240789000	2.676149000	-0.001393000
C	-1.205680000	4.086311000	-0.029908000
C	-0.000012000	4.787782000	-0.042887000
C	1.205678000	4.086347000	-0.029903000
C	0.000028000	1.924549000	0.020548000
C	1.240824000	2.676188000	-0.001388000
C	2.451540000	1.974154000	0.004468000
C	3.458256000	1.273726000	0.007597000
C	4.562450000	0.421572000	0.010744000
C	5.899473000	0.901933000	0.022390000
C	6.965459000	0.029152000	0.025311000
C	4.386432000	-1.002822000	0.004670000
C	5.494596000	-1.829184000	0.011138000
C	-7.917753000	-2.253659000	-0.024886000
C	7.917728000	-2.253692000	-0.024964000
H	-5.400235000	-2.910729000	0.007848000

H	-6.089915000	1.970958000	0.031209000
H	-7.997326000	0.364144000	0.031671000
H	-2.151896000	4.622453000	-0.043590000
H	-0.000028000	5.874068000	-0.065643000
H	2.151879000	4.622516000	-0.043581000
H	6.089963000	1.970929000	0.031251000
H	7.997338000	0.364065000	0.031717000
H	5.400161000	-2.910740000	0.007862000
H	-8.052027000	-2.623803000	-1.047481000
H	-8.817169000	-1.724464000	0.296710000
H	-7.728769000	-3.093060000	0.649966000
H	8.052670000	-2.622895000	-1.047813000
H	7.728267000	-3.093706000	0.648981000
H	8.816946000	-1.724822000	0.297729000
N	0.000060000	0.593818000	0.065744000
H	0.846557000	0.028288000	0.062346000
H	-0.846387000	0.028211000	0.062336000

2b...Cl⁻

Br	-2.673537000	-1.541508000	-0.004786000
Br	2.673548000	-1.541517000	-0.004789000
Cl	0.000006000	-2.532370000	-0.007316000
N	-6.821306000	-0.985042000	-0.011179000
N	6.821313000	-0.985025000	-0.011177000
C	-5.561630000	-1.519236000	-0.007553000
C	-4.434194000	-0.721381000	-0.003316000
C	-4.581199000	0.704225000	-0.001075000
C	-5.906520000	1.217808000	-0.004784000
C	-6.992220000	0.370316000	-0.008128000
C	-3.463322000	1.541828000	0.000801000
C	-2.452692000	2.235523000	0.001285000
C	-1.238680000	2.935083000	0.002134000
C	-1.204872000	4.345937000	0.003749000
C	0.000004000	5.048174000	0.004599000
C	1.204871000	4.345921000	0.003748000
C	-0.000013000	2.185049000	0.001186000
C	1.238663000	2.935066000	0.002133000
C	2.452670000	2.235497000	0.001282000
C	3.463308000	1.541816000	0.000797000
C	4.581192000	0.704223000	-0.001078000
C	5.906510000	1.217817000	-0.004785000
C	6.992216000	0.370334000	-0.008127000

C	4.434199000	-0.721384000	-0.003317000
C	5.561642000	-1.519230000	-0.007552000
C	-7.999433000	-1.884785000	0.042820000
C	7.999449000	-1.884757000	0.042825000
H	-5.498457000	-2.603360000	-0.009447000
H	-6.072256000	2.291187000	-0.007992000
H	-8.016668000	0.727803000	-0.009387000
H	-2.151795000	4.880937000	0.004373000
H	0.000012000	6.134710000	0.005885000
H	2.151800000	4.880908000	0.004371000
H	6.072236000	2.291198000	-0.007994000
H	8.016662000	0.727830000	-0.009385000
H	5.498478000	-2.603355000	-0.009444000
H	-7.776237000	-2.800263000	-0.510654000
H	-8.854309000	-1.382667000	-0.416112000
H	-8.229685000	-2.130189000	1.085812000
H	7.776252000	-2.800250000	-0.510624000
H	8.229719000	-2.130135000	1.085819000
H	8.854314000	-1.382643000	-0.416132000
N	-0.000030000	0.848176000	-0.000719000
H	0.858882000	0.302282000	-0.001965000
H	-0.858971000	0.302326000	-0.001965000

2c...Br⁻

I	-2.647471000	1.321767000	-0.003328000
I	2.647471000	1.321766000	-0.003328000
Br	0.000000000	2.811139000	-0.006432000
N	-6.952958000	0.370294000	-0.007807000
N	6.952958000	0.370295000	-0.007807000
C	-5.724744000	0.973648000	-0.004282000
C	-4.546766000	0.249888000	-0.001477000
C	-4.620347000	-1.180668000	-0.000351000
C	-5.913097000	-1.774200000	-0.004183000
C	-7.046558000	-0.993087000	-0.006404000
C	-3.466484000	-1.972138000	0.000741000
C	-2.452596000	-2.660355000	0.000640000
C	-1.237222000	-3.360767000	0.000729000
C	-1.204844000	-4.771899000	-0.000017000
C	0.000000000	-5.474043000	-0.000301000
C	1.204844000	-4.771899000	-0.000017000
C	0.000000000	-2.615154000	0.001332000
C	1.237222000	-3.360767000	0.000729000

C	2.452596000	-2.660355000	0.000640000
C	3.466484000	-1.972138000	0.000741000
C	4.620347000	-1.180668000	-0.000351000
C	5.913098000	-1.774200000	-0.004183000
C	7.046558000	-0.993087000	-0.006404000
C	4.546766000	0.249888000	-0.001477000
C	5.724744000	0.973648000	-0.004282000
C	-8.185224000	1.194104000	0.045478000
C	8.185224000	1.194105000	0.045478000
H	-5.733556000	2.060052000	-0.005268000
H	-6.015100000	-2.855699000	-0.008260000
H	-8.048942000	-1.408902000	-0.007844000
H	-2.151972000	-5.306437000	-0.000408000
H	0.000000000	-6.560614000	-0.000868000
H	2.151972000	-5.306437000	-0.000408000
H	6.015100000	-2.855699000	-0.008260000
H	8.048942000	-1.408902000	-0.007844000
H	5.733555000	2.060052000	-0.005268000
H	-8.510165000	1.306694000	1.086061000
H	-8.970437000	0.704604000	-0.536462000
H	-7.975835000	2.176987000	-0.382600000
H	8.510166000	1.306693000	1.086062000
H	7.975834000	2.176988000	-0.382598000
H	8.970436000	0.704606000	-0.536463000
N	0.000000000	-1.273490000	0.002485000
H	0.867939000	-0.739976000	0.001749000
H	-0.867939000	-0.739976000	0.001749000

2...Cl⁻

I	2.465014000	-1.401097000	-0.003472000
I	-2.465014000	-1.401097000	-0.003471000
Cl	0.000000000	-2.845935000	-0.006909000
N	6.804874000	-0.668458000	-0.006900000
N	-6.804874000	-0.668458000	-0.006900000
C	5.549041000	-1.203815000	-0.004422000
C	4.405674000	-0.417800000	-0.001909000
C	4.569346000	1.003384000	-0.000663000
C	5.886726000	1.528274000	-0.003635000
C	6.978271000	0.686118000	-0.005821000
C	3.450426000	1.853661000	0.000274000
C	2.437887000	2.534291000	0.000605000
C	1.220596000	3.258183000	0.001199000

C	1.210667000	4.674350000	0.002070000
C	0.000000000	5.367655000	0.002528000
C	-1.210667000	4.674350000	0.002071000
C	0.000000000	2.552945000	0.000800000
C	-1.220596000	3.258183000	0.001200000
C	-2.437886000	2.534291000	0.000606000
C	-3.450426000	1.853661000	0.000276000
C	-4.569346000	1.003384000	-0.000662000
C	-5.886726000	1.528273000	-0.003634000
C	-6.978271000	0.686118000	-0.005820000
C	-4.405674000	-0.417800000	-0.001909000
C	-5.549041000	-1.203815000	-0.004422000
C	7.993387000	-1.557044000	0.038141000
C	-7.993388000	-1.557043000	0.038139000
H	5.497706000	-2.289046000	-0.005647000
H	6.046445000	2.602865000	-0.006843000
H	8.002717000	1.043842000	-0.007014000
H	2.155569000	5.212166000	0.002364000
H	0.000000000	6.455335000	0.003194000
H	-2.155569000	5.212165000	0.002365000
H	-6.046444000	2.602865000	-0.006841000
H	-8.002717000	1.043842000	-0.007013000
H	-5.497706000	-2.289046000	-0.005648000
H	8.369242000	-1.615116000	1.065630000
H	8.768993000	-1.154156000	-0.618693000
H	7.706005000	-2.552825000	-0.305412000
H	-8.369261000	-1.615095000	1.065623000
H	-7.706000000	-2.552831000	-0.305390000
H	-8.768983000	-1.154168000	-0.618717000
H	0.000000000	1.465952000	0.000006000

2c...Cl⁻

I	-2.567577000	1.480376000	-0.004104000
I	2.567577000	1.480376000	-0.004104000
Cl	0.000000000	2.795175000	-0.006293000
N	-6.886426000	0.617339000	-0.009347000
N	6.886426000	0.617339000	-0.009347000
C	-5.646841000	1.196680000	-0.005742000
C	-4.482034000	0.450937000	-0.002315000
C	-4.584525000	-0.978920000	-0.000484000
C	-5.888705000	-1.546695000	-0.004141000
C	-7.006826000	-0.743908000	-0.007122000

C	-3.447285000	-1.794320000	0.001073000
C	-2.449235000	-2.505830000	0.001335000
C	-1.238291000	-3.214063000	0.001719000
C	-1.205701000	-4.624895000	0.001137000
C	0.000000000	-5.326302000	0.000971000
C	1.205701000	-4.624895000	0.001137000
C	0.000000000	-2.469665000	0.002370000
C	1.238291000	-3.214063000	0.001719000
C	2.449235000	-2.505830000	0.001334000
C	3.447285000	-1.794320000	0.001073000
C	4.584525000	-0.978920000	-0.000485000
C	5.888705000	-1.546695000	-0.004141000
C	7.006826000	-0.743908000	-0.007122000
C	4.482034000	0.450937000	-0.002315000
C	5.646841000	1.196681000	-0.005742000
C	-8.102118000	1.465299000	0.043371000
C	8.102118000	1.465299000	0.043371000
H	-5.634776000	2.282972000	-0.007187000
H	-6.011601000	-2.625990000	-0.007563000
H	-8.017117000	-1.140087000	-0.008565000
H	-2.152302000	-5.160397000	0.000750000
H	0.000000000	-6.412881000	0.000527000
H	2.152302000	-5.160397000	0.000750000
H	6.011601000	-2.625990000	-0.007564000
H	8.017117000	-1.140087000	-0.008566000
H	5.634776000	2.282972000	-0.007187000
H	-8.422334000	1.588599000	1.084215000
H	-8.898155000	0.988776000	-0.534594000
H	-7.874720000	2.442116000	-0.389416000
H	8.422333000	1.588600000	1.084216000
H	7.874720000	2.442116000	-0.389416000
H	8.898155000	0.988776000	-0.534593000
N	0.000000000	-1.129304000	0.003636000
H	0.867685000	-0.595099000	0.002787000
H	-0.867685000	-0.595099000	0.002787000

2c...I'

I	-2.735552000	-1.160856000	0.002330000
I	2.735551000	-1.160856000	0.002328000
I	0.000002000	-2.872732000	0.008329000
N	-7.028137000	-0.098171000	0.004127000
N	7.028136000	-0.098170000	0.004128000

C	-5.813937000	-0.730011000	0.001075000
C	-4.620643000	-0.033495000	-0.000277000
C	-4.659656000	1.396926000	-0.000084000
C	-5.937837000	2.021592000	0.003900000
C	-7.089296000	1.267074000	0.004356000
C	-3.486621000	2.159891000	-0.000154000
C	-2.456177000	2.822437000	0.000773000
C	-1.236031000	3.514619000	0.001396000
C	-1.203937000	4.926067000	0.002905000
C	0.000000000	5.628996000	0.003626000
C	1.203937000	4.926066000	0.002904000
C	-0.000001000	2.767998000	0.000601000
C	1.236029000	3.514619000	0.001396000
C	2.456175000	2.822436000	0.000772000
C	3.486621000	2.159893000	-0.000154000
C	4.659656000	1.396928000	-0.000082000
C	5.937837000	2.021594000	0.003912000
C	7.089296000	1.267076000	0.004366000
C	4.620642000	-0.033493000	-0.000280000
C	5.813935000	-0.730009000	0.001070000
C	-8.279828000	-0.892098000	-0.050652000
C	8.279827000	-0.892096000	-0.050657000
H	-5.848312000	-1.816086000	0.001252000
H	-6.014610000	3.105240000	0.009274000
H	-8.081622000	1.706431000	0.005569000
H	-2.151631000	5.459569000	0.003499000
H	0.000000000	6.715564000	0.004788000
H	2.151631000	5.459568000	0.003496000
H	6.014611000	3.105241000	0.009294000
H	8.081622000	1.706431000	0.005587000
H	5.848311000	-1.816085000	0.001241000
H	-8.612516000	-0.986870000	-1.090557000
H	-9.050484000	-0.390156000	0.540173000
H	-8.091336000	-1.883776000	0.366661000
H	8.091329000	-1.883787000	0.366622000
H	9.050475000	-0.390172000	0.540195000
H	8.612531000	-0.986836000	-1.090561000
N	-0.000003000	1.424713000	-0.000893000
H	0.868388000	0.892304000	-0.000347000
H	-0.868394000	0.892306000	-0.000346000

2d...Cl-

I	-2.589058000	-1.349343000	-0.007568000
I	2.589115000	-1.349311000	-0.007554000
Cl	-0.000161000	-2.658428000	-0.042572000
N	-6.930166000	-0.438558000	0.016702000
N	6.930165000	-0.438570000	0.016703000
C	-5.704371000	-1.076707000	0.011331000
C	-4.510235000	-0.317831000	0.008052000
C	-4.583064000	1.090307000	0.006945000
C	-5.875487000	1.709180000	0.005184000
C	-6.999889000	0.939393000	0.009061000
C	-3.431769000	1.895864000	0.002162000
C	-2.446785000	2.623352000	-0.001959000
C	-1.237022000	3.340369000	-0.005299000
C	-1.206181000	4.750529000	-0.010605000
C	0.000019000	5.451807000	-0.013278000
C	1.206199000	4.750511000	-0.010633000
C	-0.000014000	2.600483000	-0.002797000
C	1.237011000	3.340344000	-0.005329000
C	2.446756000	2.623310000	-0.002029000
C	3.431757000	1.895839000	0.002119000
C	4.583051000	1.090297000	0.006922000
C	5.875476000	1.709163000	0.005145000
C	6.999879000	0.939380000	0.009033000
C	4.510242000	-0.317850000	0.008051000
C	5.704375000	-1.076729000	0.011341000
C	-8.178617000	-1.226625000	0.043606000
C	8.178620000	-1.226632000	0.043635000
H	-5.962351000	2.790932000	0.000461000
H	-8.000916000	1.356418000	0.008141000
H	-2.152876000	5.285948000	-0.012430000
H	0.000027000	6.538468000	-0.017263000
H	2.152907000	5.285909000	-0.012481000
H	5.962337000	2.790916000	0.000399000
H	8.000903000	1.356412000	0.008102000
H	-8.271088000	-1.830766000	-0.867973000
H	-9.024769000	-0.539702000	0.093818000
H	-8.194989000	-1.876405000	0.926684000
H	8.271121000	-1.830767000	-0.867945000
H	8.194969000	-1.876415000	0.926709000
H	9.024766000	-0.539703000	0.093874000
N	-0.000034000	1.256151000	0.002430000

H	0.867706000	0.727262000	-0.000103000
H	-0.867792000	0.727285000	-0.000076000
N	5.690541000	-2.434498000	0.043994000
H	4.783028000	-2.889007000	-0.027317000
H	6.511945000	-2.991398000	-0.145236000
N	-5.690514000	-2.434473000	0.043942000
H	-4.782991000	-2.888969000	-0.027337000
H	-6.511923000	-2.991402000	-0.145169000

2e⁻Cl⁻

I	2.566867000	-1.086340000	0.000029000
I	-2.566873000	-1.086337000	0.000024000
Cl	-0.000001000	-2.330130000	0.000079000
N	6.928768000	-0.193626000	-0.000045000
N	-6.928767000	-0.193632000	-0.000041000
C	5.685443000	-0.765881000	-0.000022000
C	4.498318000	-0.066483000	-0.000004000
C	4.589206000	1.366986000	-0.000009000
C	5.884607000	1.955105000	-0.000028000
C	7.015133000	1.172828000	-0.000047000
C	3.444410000	2.168745000	0.000001000
C	2.448421000	2.884132000	0.000007000
C	1.238987000	3.592377000	0.000011000
C	1.205928000	5.003553000	0.000010000
C	-0.000001000	5.704483000	0.000011000
C	-1.205930000	5.003552000	0.000010000
C	0.000000000	2.847813000	0.000013000
C	-1.238989000	3.592376000	0.000011000
C	-2.448423000	2.884131000	0.000007000
C	-3.444415000	2.168748000	0.000001000
C	-4.589209000	1.366988000	-0.000009000
C	-5.884612000	1.955102000	-0.000018000
C	-7.015136000	1.172822000	-0.000033000
C	-4.498319000	-0.066480000	-0.000009000
C	-5.685440000	-0.765882000	-0.000028000
C	8.164810000	-1.023217000	-0.000099000
C	-8.164806000	-1.023227000	-0.000063000
H	5.990522000	3.035909000	-0.000028000
H	8.017853000	1.586040000	-0.000063000
H	2.152118000	5.539696000	0.000009000
H	-0.000002000	6.791001000	0.000011000
H	-2.152121000	5.539695000	0.000009000

H	-5.990532000	3.035905000	-0.000013000
H	-8.017857000	1.586030000	-0.000039000
H	8.184291000	-1.650001000	0.896541000
H	9.024514000	-0.352162000	-0.000004000
H	8.184334000	-1.649817000	-0.896868000
H	-8.184311000	-1.649937000	0.896629000
H	-8.184301000	-1.649902000	-0.896781000
H	-9.024512000	-0.352175000	-0.000054000
N	0.000001000	1.508922000	0.000016000
H	-0.867893000	0.974917000	0.000021000
H	0.867895000	0.974919000	0.000021000
N	-5.696063000	-2.266886000	-0.000034000
O	-5.710376000	-2.808830000	-1.106279000
O	-5.710300000	-2.808842000	1.106205000
N	5.696078000	-2.266885000	-0.000022000
O	5.710327000	-2.808834000	-1.106265000
O	5.710393000	-2.808836000	1.106220000

2f...Cl⁻

I	2.568790000	-1.554755000	-0.000304000
I	-2.568646000	-1.554776000	0.000230000
Cl	-0.000388000	-2.881111000	-0.000456000
N	6.904642000	-0.675257000	0.003237000
N	-6.904607000	-0.675256000	-0.002848000
C	5.647051000	-1.253531000	0.000664000
C	4.488505000	-0.522468000	-0.001583000
C	4.596595000	0.913412000	-0.006175000
C	5.882865000	1.484496000	-0.018909000
C	7.035395000	0.693166000	-0.013966000
C	3.453053000	1.726185000	-0.006582000
C	2.451031000	2.430294000	-0.005156000
C	1.237434000	3.137741000	-0.002658000
C	1.205314000	4.547985000	-0.002516000
C	0.000020000	5.250248000	-0.000049000
C	-1.205299000	4.547995000	0.002464000
C	-0.000004000	2.393323000	0.000028000
C	-1.237427000	3.137757000	0.002688000
C	-2.451097000	2.430408000	0.005205000
C	-3.453130000	1.726328000	0.006591000
C	-4.596668000	0.913526000	0.006196000
C	-5.882957000	1.484555000	0.018712000
C	-7.035443000	0.693160000	0.013921000

C	-4.488452000	-0.522346000	0.001896000
C	-5.646982000	-1.253454000	-0.000126000
C	8.102548000	-1.538341000	0.039900000
C	-8.102465000	-1.538420000	-0.039157000
H	5.646654000	-2.339185000	0.003612000
H	5.994819000	2.565569000	-0.034090000
H	2.152307000	5.082967000	-0.004304000
H	0.000025000	6.336900000	-0.000048000
H	-2.152276000	5.083002000	0.004232000
H	-5.994972000	2.565627000	0.033602000
H	-5.646538000	-2.339112000	-0.002736000
H	8.724555000	-1.278622000	0.904140000
H	8.683140000	-1.431499000	-0.885557000
H	7.779831000	-2.576520000	0.130562000
H	-7.779691000	-2.576612000	-0.129463000
H	-8.724519000	-1.279059000	-0.903472000
H	-8.683028000	-1.431268000	0.886281000
N	-0.000013000	1.052208000	0.000045000
H	-0.867573000	0.517678000	0.001768000
H	0.867544000	0.517687000	-0.001183000
N	-8.296792000	1.233769000	-0.038584000
H	-8.365800000	2.236293000	0.093796000
H	-9.091172000	0.708208000	0.305536000
N	8.296708000	1.233862000	0.038265000
H	8.365669000	2.236347000	-0.094439000
H	9.091113000	0.708214000	-0.305660000

2g...Cl⁻

I	-2.568314000	-1.678353000	-0.024889000
I	2.568316000	-1.678496000	-0.025122000
Cl	0.000125000	-2.971272000	-0.047944000
N	-6.898295000	-0.839395000	-0.009123000
N	6.898321000	-0.839333000	-0.009227000
C	-5.644686000	-1.396425000	-0.030348000
C	-4.478064000	-0.653283000	-0.015994000
C	-4.577601000	0.777234000	-0.010387000
C	-5.879835000	1.339345000	-0.012528000
C	-6.992370000	0.527841000	0.006484000
C	-3.445483000	1.596332000	-0.006896000
C	-2.447823000	2.309211000	-0.006762000
C	-1.238986000	3.017652000	-0.006312000
C	-1.206185000	4.429018000	-0.008986000

C	-0.000016000	5.129540000	-0.009939000
C	1.206158000	4.429011000	-0.008857000
C	-0.000012000	2.273099000	-0.003872000
C	1.238960000	3.017655000	-0.006189000
C	2.447796000	2.309200000	-0.006540000
C	3.445422000	1.596278000	-0.006741000
C	4.577558000	0.777189000	-0.010332000
C	5.879764000	1.339360000	-0.012355000
C	6.992343000	0.527905000	0.006567000
C	4.478071000	-0.653328000	-0.016136000
C	5.644734000	-1.396406000	-0.030559000
C	-8.080720000	-1.749908000	-0.068978000
C	8.080778000	-1.749803000	-0.069139000
H	-5.626753000	-2.481365000	-0.068898000
H	-6.024935000	2.414853000	-0.018308000
H	-2.152283000	4.965252000	-0.010771000
H	-0.000012000	6.216037000	-0.012259000
H	2.152254000	4.965250000	-0.010533000
H	6.024818000	2.414873000	-0.017972000
H	5.626849000	-2.481343000	-0.069251000
H	-8.796109000	-1.382248000	-0.807667000
H	-8.560895000	-1.800167000	0.910076000
H	-7.715252000	-2.732830000	-0.371264000
H	7.715343000	-2.732708000	-0.371517000
H	8.560932000	-1.800130000	0.909922000
H	8.796178000	-1.382055000	-0.807772000
N	-0.000004000	0.933578000	0.001170000
H	0.867770000	0.399478000	-0.000993000
H	-0.867770000	0.399466000	-0.001081000
N	8.332352000	1.169660000	0.102756000
O	9.178257000	0.610899000	0.814426000
O	8.470878000	2.233192000	-0.507612000
N	-8.332410000	1.169553000	0.102576000
O	-9.178279000	0.610859000	0.814337000
O	-8.470977000	2.232990000	-0.507944000

2h...Cl-

I	-2.558309000	-1.647276000	0.000541000
I	2.558309000	-1.647274000	0.000546000
Cl	-0.000001000	-2.984799000	0.016153000
N	-6.860575000	-0.778408000	-0.009865000
N	6.860574000	-0.778410000	-0.009863000

C	-5.637006000	-1.371983000	-0.012836000
C	-4.472109000	-0.614696000	-0.005394000
C	-4.561744000	0.800059000	0.001746000
C	-5.868700000	1.409883000	0.003613000
C	-6.991493000	0.579480000	-0.000050000
C	-3.424141000	1.620396000	0.009048000
C	-2.448187000	2.362519000	0.006795000
C	-1.237048000	3.076555000	0.002627000
C	-1.205121000	4.486294000	-0.014318000
C	0.000000000	5.188516000	-0.022336000
C	1.205121000	4.486295000	-0.014319000
C	0.000001000	2.332239000	0.011961000
C	1.237049000	3.076556000	0.002625000
C	2.448188000	2.362520000	0.006791000
C	3.424141000	1.620396000	0.009043000
C	4.561744000	0.800059000	0.001743000
C	5.868701000	1.409883000	0.003607000
C	6.991494000	0.579478000	-0.000055000
C	4.472108000	-0.614695000	-0.005390000
C	5.637005000	-1.371985000	-0.012830000
C	-8.092039000	-1.605739000	-0.019382000
C	8.092038000	-1.605742000	-0.019378000
H	-5.627620000	-2.456711000	-0.019856000
H	-8.004588000	0.968701000	-0.001175000
H	-2.150547000	5.024092000	-0.023483000
H	-0.000001000	6.275029000	-0.036346000
H	2.150546000	5.024093000	-0.023485000
H	8.004590000	0.968698000	-0.001180000
H	5.627618000	-2.456712000	-0.019844000
H	-8.671976000	-1.386219000	-0.921828000
H	-8.689457000	-1.380728000	0.870123000
H	-7.809954000	-2.659852000	-0.013205000
H	7.809952000	-2.659854000	-0.013193000
H	8.689458000	-1.380725000	0.870123000
H	8.671971000	-1.386228000	-0.921828000
N	0.000001000	0.989610000	0.028360000
H	0.866838000	0.454637000	0.027862000
H	-0.866835000	0.454636000	0.027863000
N	5.991859000	2.771574000	-0.026889000
H	5.161680000	3.329916000	0.136844000
H	6.885474000	3.210356000	0.154809000
N	-5.991859000	2.771580000	-0.026899000

H	-5.161682000	3.329905000	0.136918000
H	-6.885464000	3.210344000	0.154903000

2i...Cl-

I	2.598068000	-1.878361000	-0.014574000
I	-2.598032000	-1.878307000	-0.014579000
Cl	0.000052000	-3.132872000	-0.018106000
N	6.926857000	-1.099265000	0.026366000
N	-6.926828000	-1.099338000	0.026427000
C	5.664300000	-1.645485000	0.006271000
C	4.526436000	-0.869365000	-0.003313000
C	4.645194000	0.571813000	-0.004323000
C	5.980665000	1.078002000	0.019362000
C	7.083549000	0.244231000	0.039546000
C	3.506148000	1.369298000	-0.008028000
C	2.452037000	1.998222000	-0.008113000
C	1.241066000	2.693971000	-0.013288000
C	1.207345000	4.106949000	-0.035301000
C	-0.000036000	4.806096000	-0.045247000
C	-1.207397000	4.106927000	-0.035309000
C	0.000001000	1.950610000	-0.000046000
C	-1.241079000	2.693939000	-0.013294000
C	-2.452036000	1.998174000	-0.008102000
C	-3.506186000	1.369310000	-0.008006000
C	-4.645219000	0.571815000	-0.004306000
C	-5.980709000	1.077966000	0.019366000
C	-7.083564000	0.244149000	0.039549000
C	-4.526417000	-0.869364000	-0.003287000
C	-5.664254000	-1.645518000	0.006344000
C	8.107931000	-2.000361000	0.024145000
C	-8.107871000	-2.000474000	0.024252000
H	5.624773000	-2.731043000	-0.000027000
H	8.089018000	0.647723000	0.067769000
H	2.154990000	4.640480000	-0.045351000
H	-0.000045000	5.892550000	-0.062100000
H	-2.155055000	4.640433000	-0.045349000
H	-8.089043000	0.647617000	0.067727000
H	-5.624689000	-2.731075000	0.000100000
H	8.042979000	-2.681157000	0.878590000
H	9.014694000	-1.397955000	0.102161000
H	8.124018000	-2.574302000	-0.908094000
H	-8.042857000	-2.681274000	0.878689000

H	-8.123979000	-2.574410000	-0.907990000
H	-9.014650000	-1.398099000	0.102313000
N	0.000021000	0.615859000	0.022219000
H	-0.868701000	0.081538000	0.024335000
H	0.868754000	0.081558000	0.024342000
N	-6.281434000	2.539438000	0.025749000
O	-7.442141000	2.873267000	0.308593000
O	-5.357735000	3.309250000	-0.255087000
N	6.281329000	2.539487000	0.025770000
O	7.441864000	2.873369000	0.309256000
O	5.357758000	3.309231000	-0.255654000

2j...Cl-

I	2.578106000	-1.748852000	-0.004827000
I	-2.578106000	-1.748860000	-0.003530000
Cl	0.000012000	-3.059261000	-0.003937000
N	6.900850000	-0.903895000	-0.011767000
N	-6.900836000	-0.903880000	-0.013668000
C	5.653266000	-1.475535000	-0.007287000
C	4.495645000	-0.726032000	-0.003762000
C	4.598452000	0.708885000	-0.001953000
C	5.912138000	1.265763000	-0.005690000
C	7.024129000	0.458159000	-0.008509000
C	3.467516000	1.519856000	-0.000398000
C	2.444189000	2.206186000	0.000228000
C	1.244234000	2.903030000	0.001707000
C	1.218313000	4.345610000	0.001028000
C	-0.000011000	5.036786000	0.001390000
C	-1.218316000	4.345603000	0.002100000
C	0.000003000	2.180065000	0.003308000
C	-1.244231000	2.903027000	0.003078000
C	-2.444182000	2.206176000	0.003374000
C	-3.467503000	1.519836000	0.003282000
C	-4.598440000	0.708874000	-0.000070000
C	-5.912115000	1.265768000	-0.005535000
C	-7.024107000	0.458175000	-0.010173000
C	-4.495643000	-0.726041000	-0.002660000
C	-5.653264000	-1.475534000	-0.007940000
C	8.106121000	-1.761708000	0.047945000
C	-8.106194000	-1.761697000	0.044144000
H	5.635290000	-2.561819000	-0.008519000
H	6.046542000	2.343679000	-0.009313000

H	8.035670000	0.851221000	-0.009530000
H	-0.000015000	6.125305000	0.000743000
H	-6.046495000	2.343685000	-0.009638000
H	-8.035641000	0.851246000	-0.012702000
H	-5.635293000	-2.561817000	-0.009756000
H	8.363071000	-1.974492000	1.092321000
H	8.938605000	-1.246573000	-0.438001000
H	7.905692000	-2.698637000	-0.477960000
H	-8.364556000	-1.974824000	1.088102000
H	-7.905071000	-2.698455000	-0.481800000
H	-8.938016000	-1.246391000	-0.442755000
N	0.000005000	0.840405000	0.005012000
H	-0.867556000	0.305870000	0.004253000
H	0.867566000	0.305870000	0.004175000
N	-2.399578000	5.019744000	-0.004926000
H	-2.424273000	6.029596000	0.027995000
H	-3.275076000	4.513337000	0.027595000
N	2.399542000	5.019751000	0.006198000
H	2.424313000	6.029658000	-0.024624000
H	3.275158000	4.513327000	-0.022291000

2k...Cl⁻

I	2.526470000	-2.260771000	0.028604000
I	-2.526473000	-2.260770000	0.028607000
Cl	0.000006000	-3.615620000	0.081909000
N	6.839636000	-1.349531000	-0.030917000
N	-6.839635000	-1.349532000	-0.030919000
C	5.613878000	-1.950067000	-0.013826000
C	4.435065000	-1.220088000	-0.004123000
C	4.523153000	0.205179000	-0.013231000
C	5.812347000	0.800462000	-0.031453000
C	6.942948000	0.013313000	-0.040555000
C	3.376728000	1.014439000	-0.005620000
C	2.438755000	1.798406000	-0.018144000
C	1.248699000	2.539895000	-0.020739000
C	1.192830000	3.951265000	-0.007835000
C	0.000000000	4.662408000	0.020539000
C	-1.192830000	3.951265000	-0.007836000
C	0.000000000	1.808407000	0.000909000
C	-1.248699000	2.539895000	-0.020739000
C	-2.438754000	1.798406000	-0.018145000
C	-3.376727000	1.014439000	-0.005621000

C	-4.523152000	0.205178000	-0.013232000
C	-5.812346000	0.800461000	-0.031459000
C	-6.942947000	0.013313000	-0.040561000
C	-4.435065000	-1.220088000	-0.004121000
C	-5.613877000	-1.950068000	-0.013824000
C	8.075284000	-2.172234000	-0.080140000
C	-8.075285000	-2.172232000	-0.080133000
H	5.619012000	-3.036309000	-0.006829000
H	5.911398000	1.882485000	-0.038825000
H	7.948075000	0.422325000	-0.056421000
H	0.000000000	5.745549000	0.060693000
H	-5.911398000	1.882485000	-0.038835000
H	-7.948074000	0.422324000	-0.056432000
H	-5.619011000	-3.036310000	-0.006823000
H	7.830068000	-3.199219000	0.197195000
H	8.805586000	-1.767290000	0.625932000
H	8.487520000	-2.151888000	-1.094881000
H	-7.830056000	-3.199234000	0.197124000
H	-8.487572000	-2.151821000	-1.094852000
H	-8.805553000	-1.767334000	0.626000000
N	0.000000000	0.468365000	0.034583000
H	-0.869230000	-0.064120000	0.039913000
H	0.869231000	-0.064120000	0.039913000
N	-2.454633000	4.749506000	-0.016827000
O	-3.460572000	4.224128000	-0.516040000
O	-2.403049000	5.883358000	0.472797000
N	2.454634000	4.749506000	-0.016824000
O	3.460571000	4.224131000	-0.516043000
O	2.403050000	5.883354000	0.472807000

2|...Cl-

I	2.564711000	-1.665663000	-0.013918000
I	-2.564712000	-1.665664000	-0.013919000
Cl	0.000001000	-2.990263000	-0.040535000
N	6.882275000	-0.798578000	0.017336000
N	-6.882276000	-0.798577000	0.017336000
C	5.641525000	-1.378390000	0.010591000
C	4.477274000	-0.633454000	0.004303000
C	4.577586000	0.797531000	0.007339000
C	5.882998000	1.365324000	0.014513000
C	7.001111000	0.563685000	0.020961000
C	3.441242000	1.612415000	0.000611000

C	2.444517000	2.326819000	-0.003683000
C	1.233609000	3.033522000	-0.006066000
C	1.204714000	4.442426000	-0.007882000
C	0.000000000	5.165389000	-0.009273000
C	-1.204714000	4.442427000	-0.007881000
C	0.000000000	2.283578000	-0.005821000
C	-1.233608000	3.033521000	-0.006065000
C	-2.444516000	2.326818000	-0.003682000
C	-3.441241000	1.612414000	0.000613000
C	-4.577585000	0.797531000	0.007341000
C	-5.882997000	1.365325000	0.014516000
C	-7.001110000	0.563686000	0.020964000
C	-4.477275000	-0.633455000	0.004302000
C	-5.641526000	-1.378390000	0.010589000
C	8.096372000	-1.646212000	0.082925000
C	-8.096373000	-1.646210000	0.082924000
H	5.629927000	-2.464679000	0.008962000
H	6.005704000	2.444648000	0.012530000
H	8.011061000	0.960637000	0.028402000
H	2.154197000	4.974536000	-0.002602000
H	-2.154198000	4.974535000	-0.002601000
H	-6.005702000	2.444648000	0.012536000
H	-8.011060000	0.960639000	0.028408000
H	-5.629929000	-2.464679000	0.008956000
H	8.396715000	-1.784674000	1.127962000
H	8.903838000	-1.161749000	-0.472197000
H	7.878850000	-2.617178000	-0.368097000
H	-8.396718000	-1.784672000	1.127960000
H	-7.878851000	-2.617176000	-0.368098000
H	-8.903838000	-1.161747000	-0.472199000
N	0.000000000	0.941092000	-0.005403000
H	-0.867730000	0.407348000	-0.006319000
H	0.867730000	0.407349000	-0.006318000
N	0.000001000	6.559726000	0.059729000
H	-0.844308000	7.026794000	-0.254343000
H	0.844311000	7.026793000	-0.254341000

2m...Cl⁻

I	2.573657000	-1.981472000	0.003491000
I	-2.573659000	-1.981471000	0.003492000
Cl	0.000008000	-3.275050000	0.005116000
N	6.893759000	-1.120080000	0.008780000

N	-6.893758000	-1.120083000	0.008777000
C	5.656844000	-1.701349000	0.005434000
C	4.490046000	-0.955846000	0.002225000
C	4.594205000	0.471840000	0.000768000
C	5.894899000	1.043041000	0.004254000
C	7.014342000	0.240572000	0.007133000
C	3.453134000	1.286820000	-0.000551000
C	2.455052000	1.994873000	-0.000836000
C	1.241394000	2.704848000	-0.001245000
C	1.216684000	4.108314000	-0.001004000
C	-0.000001000	4.788554000	-0.000996000
C	-1.216685000	4.108313000	-0.001003000
C	0.000001000	1.961146000	-0.001648000
C	-1.241393000	2.704847000	-0.001244000
C	-2.455051000	1.994870000	-0.000834000
C	-3.453132000	1.286818000	-0.000546000
C	-4.594204000	0.471838000	0.000772000
C	-5.894898000	1.043038000	0.004256000
C	-7.014341000	0.240569000	0.007132000
C	-4.490045000	-0.955849000	0.002225000
C	-5.656843000	-1.701352000	0.005431000
C	8.113337000	-1.965137000	-0.039316000
C	-8.113338000	-1.965138000	-0.039318000
H	5.645963000	-2.787608000	0.006674000
H	6.016181000	2.122557000	0.007476000
H	8.024462000	0.637205000	0.008678000
H	2.143687000	4.672932000	-0.000782000
H	-2.143689000	4.672929000	-0.000780000
H	-6.016180000	2.122554000	0.007479000
H	-8.024461000	0.637202000	0.008676000
H	-5.645962000	-2.787611000	0.006670000
H	7.873924000	-2.958177000	0.346888000
H	8.889988000	-1.510642000	0.581311000
H	8.464133000	-2.045763000	-1.074240000
H	-7.873912000	-2.958194000	0.346834000
H	-8.464165000	-2.045718000	-1.074235000
H	-8.889970000	-1.510670000	0.581353000
N	0.000002000	0.624290000	-0.002393000
H	-0.868251000	0.088858000	-0.001771000
H	0.868257000	0.088859000	-0.001772000
N	-0.000002000	6.269989000	-0.000830000
O	1.101734000	6.841282000	-0.000773000

O	-1.101740000	6.841281000	-0.000773000
2a			
Cl	3.391036000	-2.195425000	-0.006906000
Cl	-3.391032000	-2.195428000	-0.006888000
N	7.213087000	-1.135073000	-0.012311000
N	-7.213084000	-1.135081000	-0.012311000
C	6.054879000	-1.852731000	-0.008841000
C	4.824670000	-1.219735000	-0.004115000
C	4.738015000	0.206193000	-0.000884000
C	5.976124000	0.906564000	-0.002736000
C	7.175399000	0.230576000	-0.007769000
C	3.514415000	0.878143000	0.000309000
C	2.457786000	1.499506000	0.000704000
C	1.234463000	2.185215000	0.001326000
C	1.203709000	3.599415000	0.002266000
C	-0.000001000	4.301113000	0.002758000
C	-1.203711000	3.599415000	0.002267000
C	-0.000001000	1.443884000	0.000897000
C	-1.234464000	2.185215000	0.001328000
C	-2.457786000	1.499506000	0.000708000
C	-3.514414000	0.878141000	0.000314000
C	-4.738013000	0.206189000	-0.000881000
C	-5.976125000	0.906559000	-0.002741000
C	-7.175397000	0.230570000	-0.007776000
C	-4.824667000	-1.219738000	-0.004106000
C	-6.054877000	-1.852736000	-0.008834000
C	8.522941000	-1.843008000	0.033747000
C	-8.522952000	-1.842990000	0.033731000
H	6.144191000	-2.934184000	-0.010679000
H	5.979289000	1.992320000	-0.003580000
H	8.133951000	0.739822000	-0.008877000
H	2.150408000	4.134222000	0.002591000
H	-0.000001000	5.387512000	0.003473000
H	-2.150410000	4.134221000	0.002593000
H	-5.979290000	1.992315000	-0.003589000
H	-8.133952000	0.739813000	-0.008890000
H	-6.144184000	-2.934190000	-0.010667000
H	8.839295000	-1.953202000	1.076792000
H	9.260901000	-1.258490000	-0.520558000
H	8.413586000	-2.826180000	-0.429030000
H	-8.839582000	-1.952691000	1.076744000

H	-8.413475000	-2.826381000	-0.428547000
H	-9.260765000	-1.258734000	-0.521049000
N	0.000000000	0.093379000	0.000171000
H	-0.872454000	-0.422915000	-0.000549000
H	0.872454000	-0.422914000	-0.000548000

2b

Br	-3.254567000	-1.947102000	-0.003758000
Br	3.254568000	-1.947104000	-0.003759000
N	-7.208439000	-0.774983000	-0.010695000
N	7.208439000	-0.774981000	-0.010695000
C	-6.051036000	-1.494648000	-0.006408000
C	-4.819816000	-0.864529000	-0.002247000
C	-4.729411000	0.560517000	-0.000433000
C	-5.967383000	1.263959000	-0.003208000
C	-7.167689000	0.591241000	-0.007811000
C	-3.509083000	1.237862000	0.000692000
C	-2.456874000	1.866744000	0.000993000
C	-1.234478000	2.553393000	0.001392000
C	-1.203735000	3.967537000	0.001540000
C	-0.000001000	4.669249000	0.001675000
C	1.203733000	3.967537000	0.001541000
C	-0.000001000	1.811720000	0.001477000
C	1.234476000	2.553394000	0.001393000
C	2.456873000	1.866744000	0.000996000
C	3.509082000	1.237861000	0.000694000
C	4.729411000	0.560516000	-0.000432000
C	5.967382000	1.263959000	-0.003206000
C	7.167688000	0.591243000	-0.007809000
C	4.819817000	-0.864530000	-0.002247000
C	6.051038000	-1.494647000	-0.006408000
C	-8.522629000	-1.474936000	0.030966000
C	8.522631000	-1.474932000	0.030963000
H	-6.147606000	-2.575350000	-0.007118000
H	-5.967619000	2.349804000	-0.004869000
H	-8.125381000	1.102378000	-0.009705000
H	-2.150435000	4.502352000	0.001532000
H	-0.000001000	5.755648000	0.001802000
H	2.150433000	4.502352000	0.001534000
H	5.967617000	2.349805000	-0.004866000
H	8.125380000	1.102381000	-0.009703000
H	6.147608000	-2.575350000	-0.007119000

H	-8.394461000	-2.496019000	-0.333748000
H	-9.228480000	-0.943051000	-0.611962000
H	-8.892671000	-1.490285000	1.061894000
H	8.394459000	-2.496022000	-0.333728000
H	8.892686000	-1.490260000	1.061887000
H	9.228473000	-0.943059000	-0.611984000
N	-0.000001000	0.461511000	0.001623000
H	0.872883000	-0.055227000	0.001460000
H	-0.872884000	-0.055228000	0.001459000

2

I	3.379633000	-1.849256000	0.001452000
I	-3.379633000	-1.849256000	-0.001451000
N	7.385940000	-0.224081000	0.009376000
N	-7.385940000	-0.224081000	-0.009377000
C	6.290990000	-1.033422000	0.005356000
C	5.004893000	-0.511543000	0.002382000
C	4.814373000	0.903367000	0.002345000
C	5.987204000	1.705826000	0.005502000
C	7.240150000	1.133282000	0.008790000
C	3.544950000	1.501176000	0.001624000
C	2.459301000	2.061406000	0.001222000
C	1.220441000	2.748247000	0.000605000
C	1.208815000	4.166875000	0.000623000
C	0.000000000	4.861425000	0.000000000
C	-1.208816000	4.166875000	-0.000622000
C	0.000000000	2.042039000	0.000000000
C	-1.220442000	2.748247000	-0.000605000
C	-2.459301000	2.061406000	-0.001221000
C	-3.544950000	1.501176000	-0.001624000
C	-4.814374000	0.903368000	-0.002346000
C	-5.987204000	1.705826000	-0.005503000
C	-7.240150000	1.133281000	-0.008791000
C	-5.004894000	-0.511543000	-0.002383000
C	-6.290990000	-1.033422000	-0.005358000
C	8.754585000	-0.813458000	-0.022019000
C	-8.754584000	-0.813460000	0.022018000
H	6.482075000	-2.101516000	0.005068000
H	5.899082000	2.788189000	0.007767000
H	8.154489000	1.718538000	0.011044000
H	2.153081000	4.705459000	0.001101000
H	0.000000000	5.948831000	0.000001000

H	-2.153081000	4.705459000	-0.001101000
H	-5.899083000	2.788190000	-0.007767000
H	-8.154489000	1.718538000	-0.011046000
H	-6.482076000	-2.101516000	-0.005069000
H	9.381952000	-0.294489000	0.707650000
H	9.173327000	-0.697872000	-1.027315000
H	8.692261000	-1.872372000	0.235029000
H	-9.173314000	-0.697903000	1.027323000
H	-8.692263000	-1.872366000	-0.235061000
H	-9.381961000	-0.294470000	-0.707628000
H	0.000000000	0.955750000	0.000000000

2c

I	3.198338000	-1.817587000	-0.002676000
I	-3.198337000	-1.817585000	-0.002676000
N	7.276594000	-0.376462000	-0.005723000
N	-7.276595000	-0.376463000	-0.005726000
C	6.143287000	-1.134047000	-0.003018000
C	4.887142000	-0.551340000	-0.000860000
C	4.754561000	0.871903000	0.000061000
C	5.968046000	1.618506000	-0.001631000
C	7.190362000	0.988107000	-0.004202000
C	3.517806000	1.520091000	0.000329000
C	2.459237000	2.138516000	0.000198000
C	1.234326000	2.821174000	0.000179000
C	1.203530000	4.235344000	-0.000099000
C	0.000000000	4.937248000	-0.000220000
C	-1.203531000	4.235344000	-0.000099000
C	-0.000001000	2.079476000	0.000401000
C	-1.234327000	2.821174000	0.000179000
C	-2.459237000	2.138517000	0.000199000
C	-3.517806000	1.520092000	0.000329000
C	-4.754562000	0.871903000	0.000060000
C	-5.968047000	1.618506000	-0.001633000
C	-7.190363000	0.988106000	-0.004205000
C	-4.887142000	-0.551340000	-0.000860000
C	-6.143287000	-1.134048000	-0.003020000
C	8.616483000	-1.025887000	0.025153000
C	-8.616482000	-1.025892000	0.025159000
H	6.284551000	-2.209848000	-0.003187000
H	5.930830000	2.703792000	-0.003143000
H	8.130547000	1.531028000	-0.005252000

H	2.150288000	4.770044000	-0.000226000
H	0.000000000	6.023652000	-0.000442000
H	-2.150289000	4.770044000	-0.000226000
H	-5.930833000	2.703792000	-0.003145000
H	-8.130548000	1.531027000	-0.005255000
H	-6.284552000	-2.209849000	-0.003189000
H	9.052961000	-0.907713000	1.022641000
H	9.258948000	-0.553574000	-0.723168000
H	8.503918000	-2.086535000	-0.206659000
H	-9.052916000	-0.907795000	1.022675000
H	-8.503926000	-2.086522000	-0.206741000
H	-9.258979000	-0.553522000	-0.723097000
N	-0.000001000	0.729380000	0.000866000
H	-0.872870000	0.211111000	0.000877000
H	0.872868000	0.211111000	0.000877000

2d

I	-3.350132000	-1.718580000	-0.000005000
I	3.350132000	-1.718580000	0.000000000
N	-7.395267000	-0.082054000	0.000006000
N	7.395267000	-0.082054000	0.000004000
C	-6.316802000	-0.945303000	0.000002000
C	-5.006665000	-0.399653000	0.000000000
C	-4.799127000	0.994211000	0.000002000
C	-5.958785000	1.834406000	0.000005000
C	-7.204665000	1.282020000	0.000007000
C	-3.527430000	1.584083000	0.000001000
C	-2.462079000	2.188195000	0.000000000
C	-1.232550000	2.869243000	-0.000001000
C	-1.203233000	4.282792000	-0.000003000
C	0.000000000	4.985173000	-0.000004000
C	1.203233000	4.282791000	-0.000004000
C	0.000000000	2.130512000	-0.000001000
C	1.232550000	2.869243000	-0.000003000
C	2.462079000	2.188194000	-0.000002000
C	3.527430000	1.584082000	-0.000002000
C	4.799127000	0.994210000	-0.000001000
C	5.958784000	1.834406000	0.000001000
C	7.204665000	1.282020000	0.000003000
C	5.006665000	-0.399653000	0.000001000
C	6.316802000	-0.945303000	0.000003000
C	-8.776191000	-0.620743000	0.000009000

C	8.776191000	-0.620742000	0.000005000
H	-5.845300000	2.913188000	0.000006000
H	-8.109571000	1.879913000	0.000010000
H	-2.150433000	4.816680000	-0.000002000
H	0.000000000	6.071600000	-0.000005000
H	2.150434000	4.816680000	-0.000005000
H	5.845300000	2.913188000	0.000001000
H	8.109571000	1.879913000	0.000004000
H	-8.947040000	-1.222289000	-0.900773000
H	-9.474728000	0.216825000	0.000018000
H	-8.947032000	-1.222300000	0.900786000
H	8.947037000	-1.222294000	-0.900775000
H	8.947035000	-1.222295000	0.900785000
H	9.474728000	0.216825000	0.000007000
N	-0.000001000	0.776348000	-0.000001000
H	0.873183000	0.261569000	0.000004000
H	-0.873184000	0.261569000	0.000005000
N	6.560352000	-2.274042000	0.000003000
H	5.778451000	-2.920486000	0.000005000
H	7.493758000	-2.661244000	0.000011000
N	-6.560350000	-2.274042000	0.000003000
H	-5.778448000	-2.920485000	-0.000004000
H	-7.493756000	-2.661246000	-0.000007000

2e

I	-3.210466000	-1.408715000	0.000028000
I	3.210467000	-1.408714000	-0.000004000
N	-7.312851000	0.061947000	-0.000004000
N	7.312850000	0.061946000	-0.000014000
C	-6.174913000	-0.690095000	0.000007000
C	-4.902094000	-0.149656000	0.000007000
C	-4.763187000	1.276576000	-0.000004000
C	-5.966389000	2.038629000	-0.000016000
C	-7.196830000	1.426707000	-0.000016000
C	-3.520712000	1.910805000	-0.000003000
C	-2.459861000	2.526505000	-0.000004000
C	-1.234960000	3.207195000	-0.000011000
C	-1.203603000	4.621868000	-0.000017000
C	0.000000000	5.323520000	-0.000023000
C	1.203603000	4.621868000	-0.000024000
C	0.000000000	2.465132000	-0.000012000
C	1.234960000	3.207195000	-0.000019000

C	2.459862000	2.526505000	-0.000020000
C	3.520713000	1.910805000	-0.000020000
C	4.763187000	1.276576000	-0.000018000
C	5.966389000	2.038628000	-0.000023000
C	7.196830000	1.426706000	-0.000021000
C	4.902094000	-0.149656000	-0.000012000
C	6.174912000	-0.690095000	-0.000010000
C	-8.663077000	-0.579535000	0.000009000
C	8.663076000	-0.579536000	-0.000008000
H	-5.915643000	3.123150000	-0.000026000
H	-8.128082000	1.983313000	-0.000025000
H	-2.150067000	5.157073000	-0.000016000
H	0.000000000	6.409919000	-0.000027000
H	2.150067000	5.157073000	-0.000029000
H	5.915644000	3.123149000	-0.000028000
H	8.128082000	1.983312000	-0.000024000
H	-8.772091000	-1.194024000	-0.898609000
H	-9.412339000	0.212613000	-0.000062000
H	-8.772129000	-1.193907000	0.898702000
H	8.772105000	-1.193984000	-0.898652000
H	8.772113000	-1.193949000	0.898659000
H	9.412338000	0.212611000	-0.000027000
N	0.000000000	1.116085000	-0.000006000
H	0.872924000	0.597802000	-0.000007000
H	-0.872924000	0.597802000	-0.000001000
N	6.391620000	-2.174951000	-0.000003000
O	6.473168000	-2.702762000	1.108144000
O	6.473148000	-2.702777000	-1.108142000
N	-6.391622000	-2.174951000	0.000022000
O	-6.473198000	-2.702751000	1.108171000
O	-6.473121000	-2.702787000	-1.108116000

2f

I	3.094549000	-1.878369000	-0.000012000
I	-3.094545000	-1.878367000	0.000003000
N	7.226860000	-0.542990000	0.000008000
N	-7.226861000	-0.542994000	0.000007000
C	6.052678000	-1.265238000	0.000000000
C	4.823215000	-0.661484000	-0.000001000
C	4.738686000	0.775800000	0.000004000
C	5.949627000	1.486013000	0.000006000
C	7.194615000	0.835861000	0.000009000

C	3.511046000	1.451205000	0.000001000
C	2.458590000	2.077148000	0.000000000
C	1.233459000	2.764909000	-0.000003000
C	1.203567000	4.177880000	-0.000004000
C	0.000000000	4.880199000	-0.000006000
C	-1.203568000	4.177882000	-0.000008000
C	-0.000003000	2.024489000	-0.000003000
C	-1.233463000	2.764911000	-0.000006000
C	-2.458595000	2.077153000	-0.000006000
C	-3.511050000	1.451208000	-0.000006000
C	-4.738689000	0.775801000	-0.000003000
C	-5.949631000	1.486011000	-0.000002000
C	-7.194618000	0.835857000	0.000003000
C	-4.823215000	-0.661484000	0.000001000
C	-6.052677000	-1.265240000	0.000006000
C	8.522586000	-1.261371000	0.000021000
C	-8.522586000	-1.261377000	0.000014000
H	6.173109000	-2.342883000	-0.000004000
H	5.932001000	2.572115000	0.000006000
H	2.150522000	4.712271000	-0.000002000
H	0.000001000	5.966617000	-0.000006000
H	-2.150523000	4.712275000	-0.000009000
H	-5.932007000	2.572114000	-0.000004000
H	-6.173106000	-2.342885000	0.000009000
H	9.093802000	-1.005838000	0.900455000
H	9.093808000	-1.005865000	-0.900417000
H	8.327883000	-2.334577000	0.000034000
H	-8.327880000	-2.334583000	0.000029000
H	-9.093803000	-1.005871000	-0.900426000
H	-9.093806000	-1.005847000	0.900445000
N	-0.000004000	0.673014000	0.000003000
H	-0.872822000	0.154851000	-0.000010000
H	0.872813000	0.154849000	-0.000008000
N	-8.362708000	1.522323000	0.000010000
H	-8.346975000	2.534635000	-0.000016000
H	-9.269517000	1.076195000	-0.000026000
N	8.362703000	1.522328000	0.000030000
H	8.346969000	2.534640000	0.000006000
H	9.269514000	1.076203000	-0.000048000

2g

I	-3.295350000	-2.138718000	-0.028470000
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I	3.295350000	-2.138718000	-0.028460000
N	-7.348821000	-0.605531000	-0.006726000
N	7.348821000	-0.605531000	-0.006727000
C	-6.219151000	-1.377559000	-0.027762000
C	-4.947767000	-0.831225000	-0.015997000
C	-4.776027000	0.589512000	-0.008723000
C	-5.968257000	1.364082000	-0.011090000
C	-7.199603000	0.753934000	0.007410000
C	-3.527958000	1.211395000	-0.007927000
C	-2.460893000	1.816322000	-0.009216000
C	-1.234812000	2.493765000	-0.010105000
C	-1.203508000	3.908761000	-0.012279000
C	0.000000000	4.610422000	-0.013454000
C	1.203508000	3.908761000	-0.012279000
C	0.000000000	1.751058000	-0.008929000
C	1.234812000	2.493765000	-0.010105000
C	2.460893000	1.816323000	-0.009215000
C	3.527958000	1.211395000	-0.007926000
C	4.776027000	0.589512000	-0.008722000
C	5.968257000	1.364082000	-0.011093000
C	7.199603000	0.753934000	0.007407000
C	4.947768000	-0.831225000	-0.015993000
C	6.219151000	-1.377559000	-0.027759000
C	-8.685877000	-1.280153000	-0.040115000
C	8.685877000	-1.280153000	-0.040116000
H	-6.385775000	-2.448999000	-0.060495000
H	-5.922761000	2.448670000	-0.025246000
H	-2.150017000	4.443900000	-0.013425000
H	-0.000001000	5.696833000	-0.015599000
H	2.150017000	4.443901000	-0.013424000
H	5.922761000	2.448670000	-0.025251000
H	6.385775000	-2.448999000	-0.060489000
H	-9.320919000	-0.795899000	-0.785801000
H	-9.152824000	-1.211904000	0.944835000
H	-8.520433000	-2.321433000	-0.320678000
H	8.520432000	-2.321434000	-0.320675000
H	9.152826000	-1.211900000	0.944833000
H	9.320917000	-0.795901000	-0.785805000
N	0.000000000	0.401997000	-0.006150000
H	0.872679000	-0.116702000	-0.005145000
H	-0.872679000	-0.116702000	-0.005145000
N	8.422100000	1.616292000	0.089035000

O	9.269374000	1.289517000	0.924448000
O	8.437812000	2.591264000	-0.660745000
N	-8.422100000	1.616291000	0.089043000
O	-9.269372000	1.289514000	0.924456000
O	-8.437814000	2.591266000	-0.660735000

2h

I	3.049609000	-1.948475000	-0.000003000
I	-3.049609000	-1.948476000	-0.000011000
N	7.163319000	-0.663718000	-0.000012000
N	-7.163320000	-0.663718000	-0.000010000
C	6.016788000	-1.390752000	-0.000006000
C	4.785751000	-0.744420000	-0.000002000
C	4.696855000	0.667406000	-0.000001000
C	5.939557000	1.409507000	-0.000006000
C	7.144804000	0.696509000	-0.000013000
C	3.482694000	1.363802000	0.000000000
C	2.456122000	2.034639000	0.000000000
C	1.234110000	2.729900000	0.000002000
C	1.203381000	4.142292000	0.000004000
C	0.000000000	4.844544000	0.000005000
C	-1.203381000	4.142292000	0.000004000
C	0.000000000	1.989332000	0.000001000
C	-1.234110000	2.729900000	0.000002000
C	-2.456121000	2.034639000	0.000001000
C	-3.482693000	1.363802000	0.000001000
C	-4.696855000	0.667406000	0.000000000
C	-5.939557000	1.409508000	-0.000002000
C	-7.144804000	0.696510000	-0.000008000
C	-4.785751000	-0.744420000	-0.000003000
C	-6.016788000	-1.390752000	-0.000007000
C	8.483370000	-1.354692000	0.000060000
C	-8.483370000	-1.354691000	0.000064000
H	6.118897000	-2.469195000	-0.000004000
H	8.109893000	1.193275000	-0.000017000
H	2.147798000	4.681175000	0.000004000
H	0.000000000	5.930911000	0.000006000
H	-2.147798000	4.681175000	0.000005000
H	-8.109892000	1.193275000	-0.000010000
H	-6.118897000	-2.469195000	-0.000007000
H	9.039369000	-1.065821000	0.897315000
H	9.039804000	-1.065165000	-0.896709000

H	8.318930000	-2.433164000	-0.000381000
H	-8.318931000	-2.433164000	-0.000391000
H	-9.039811000	-1.065154000	-0.896697000
H	-9.039363000	-1.065831000	0.897327000
N	0.000000000	0.637609000	0.000000000
H	-0.871981000	0.118059000	-0.000002000
H	0.871982000	0.118059000	-0.000002000
N	-5.924889000	2.765900000	-0.000002000
H	-5.042059000	3.261476000	-0.000006000
H	-6.778491000	3.309416000	-0.000005000
N	5.924889000	2.765900000	-0.000009000
H	5.042060000	3.261476000	-0.000013000
H	6.778491000	3.309416000	-0.000015000

2i

I	3.437819000	-2.324528000	-0.016713000
I	-3.437825000	-2.324532000	-0.016666000
N	7.454005000	-0.722139000	0.043374000
N	-7.454007000	-0.722129000	0.043368000
C	6.340650000	-1.521838000	0.018306000
C	5.069904000	-0.985542000	0.002327000
C	4.865988000	0.440845000	-0.004105000
C	6.070300000	1.209421000	0.028896000
C	7.320838000	0.626055000	0.059185000
C	3.594775000	0.998057000	-0.015683000
C	2.466653000	1.481089000	-0.021492000
C	1.234225000	2.138760000	-0.037656000
C	1.204054000	3.555608000	-0.077726000
C	0.000001000	4.256366000	-0.098023000
C	-1.204052000	3.555609000	-0.077730000
C	0.000000000	1.396332000	-0.017518000
C	-1.234224000	2.138762000	-0.037659000
C	-2.466653000	1.481090000	-0.021497000
C	-3.594772000	0.998053000	-0.015691000
C	-4.865986000	0.440843000	-0.004114000
C	-6.070295000	1.209424000	0.028871000
C	-7.320835000	0.626065000	0.059163000
C	-5.069906000	-0.985542000	0.002337000
C	-6.340655000	-1.521833000	0.018316000
C	8.805575000	-1.352945000	0.032736000
C	-8.805579000	-1.352930000	0.032731000
H	6.523166000	-2.591726000	0.013701000

H	8.220149000	1.231590000	0.099198000
H	2.153591000	4.085534000	-0.093618000
H	0.000002000	5.342447000	-0.129278000
H	-2.153589000	4.085536000	-0.093625000
H	-8.220144000	1.231603000	0.099167000
H	-6.523175000	-2.591720000	0.013726000
H	8.853019000	-2.107448000	0.823223000
H	9.555310000	-0.581145000	0.214860000
H	8.978126000	-1.817328000	-0.943686000
H	-8.853029000	-2.107424000	0.823227000
H	-8.978128000	-1.817324000	-0.943686000
H	-9.555312000	-0.581126000	0.214843000
N	-0.000001000	0.048933000	0.017556000
H	-0.873567000	-0.468381000	0.033194000
H	0.873565000	-0.468382000	0.033197000
N	-6.052751000	2.708461000	0.037901000
O	-7.068429000	3.267321000	0.462808000
O	-5.033359000	3.258548000	-0.386620000
N	6.052764000	2.708459000	0.037943000
O	7.068459000	3.267309000	0.462821000
O	5.033360000	3.258555000	-0.386536000

2j

I	2.987190000	-2.030000000	-0.004075000
I	-2.987189000	-2.029998000	-0.004094000
N	7.143113000	-0.829848000	-0.009447000
N	-7.143114000	-0.829848000	-0.009450000
C	5.961043000	-1.515458000	-0.004777000
C	4.746478000	-0.859527000	-0.001345000
C	4.690453000	0.574766000	0.000133000
C	5.955700000	1.241485000	-0.002822000
C	7.134906000	0.539478000	-0.006607000
C	3.498571000	1.285434000	0.001087000
C	2.444380000	1.925867000	0.000869000
C	1.243145000	2.615466000	0.000923000
C	1.218678000	4.066033000	0.000425000
C	0.000000000	4.753601000	0.000238000
C	-1.218679000	4.066032000	0.000445000
C	0.000000000	1.898385000	0.001368000
C	-1.243146000	2.615466000	0.000937000
C	-2.444381000	1.925866000	0.000889000
C	-3.498572000	1.285434000	0.001108000

C	-4.690454000	0.574766000	0.000150000
C	-5.955701000	1.241485000	-0.002800000
C	-7.134906000	0.539477000	-0.006594000
C	-4.746479000	-0.859527000	-0.001347000
C	-5.961043000	-1.515458000	-0.004787000
C	8.435666000	-1.562552000	0.036975000
C	-8.435663000	-1.562558000	0.036972000
H	6.036036000	-2.597943000	-0.004962000
H	5.991372000	2.326551000	-0.005303000
H	8.105164000	1.026321000	-0.008221000
H	-0.000001000	5.841773000	-0.000149000
H	-5.991373000	2.326551000	-0.005271000
H	-8.105164000	1.026321000	-0.008204000
H	-6.036037000	-2.597943000	-0.004986000
H	8.812259000	-1.578871000	1.065783000
H	9.154836000	-1.059495000	-0.614859000
H	8.279852000	-2.584127000	-0.315978000
H	-8.812193000	-1.578990000	1.065801000
H	-8.279871000	-2.584094000	-0.316105000
H	-9.154873000	-1.059429000	-0.614762000
N	0.000000000	0.550176000	0.002250000
H	-0.872923000	0.031445000	0.002428000
H	0.872922000	0.031445000	0.002412000
N	-2.393740000	4.739099000	0.000158000
H	-2.416978000	5.750944000	0.000017000
H	-3.275055000	4.241997000	0.000669000
N	2.393739000	4.739100000	0.000123000
H	2.416977000	5.750944000	-0.000037000
H	3.275055000	4.241997000	0.000592000

2k

I	-3.447639000	-2.667561000	-0.072244000
I	3.447645000	-2.667565000	-0.072252000
N	-7.376517000	-0.859372000	0.110348000
N	7.376516000	-0.859363000	0.110351000
C	-6.326762000	-1.723799000	0.051440000
C	-5.017897000	-1.263497000	0.012971000
C	-4.759179000	0.136321000	0.033514000
C	-5.885347000	1.002569000	0.096881000
C	-7.163194000	0.490465000	0.133902000
C	-3.470302000	0.686971000	0.000182000
C	-2.450979000	1.361812000	0.007389000

C	-1.244076000	2.077469000	0.007268000
C	-1.190746000	3.490939000	-0.004785000
C	0.000000000	4.203548000	-0.035069000
C	1.190744000	3.490936000	-0.004786000
C	-0.000004000	1.349757000	-0.015654000
C	1.244070000	2.077466000	0.007267000
C	2.450972000	1.361806000	0.007387000
C	3.470296000	0.686967000	0.000183000
C	4.759175000	0.136321000	0.033518000
C	5.885340000	1.002573000	0.096888000
C	7.163188000	0.490473000	0.133909000
C	5.017898000	-1.263495000	0.012971000
C	6.326764000	-1.723793000	0.051440000
C	-8.775932000	-1.373598000	0.137327000
C	8.775932000	-1.373584000	0.137337000
H	-6.572239000	-2.780579000	0.036299000
H	-5.733606000	2.078425000	0.121263000
H	-8.047343000	1.118801000	0.183667000
H	0.000001000	5.287567000	-0.083388000
H	5.733595000	2.078429000	0.121272000
H	8.047335000	1.118812000	0.183676000
H	6.572245000	-2.780572000	0.036296000
H	-8.754415000	-2.462837000	0.198924000
H	-9.288735000	-1.063204000	-0.778650000
H	-9.288985000	-0.963812000	1.012412000
H	8.754420000	-2.462826000	0.198882000
H	9.288966000	-0.963836000	1.012452000
H	9.288754000	-1.063144000	-0.778614000
N	-0.000005000	0.000863000	-0.052216000
H	0.874169000	-0.514787000	-0.058998000
H	-0.874181000	-0.514785000	-0.058997000
N	2.458490000	4.287096000	-0.006620000
O	3.440813000	3.790546000	0.564664000
O	2.423841000	5.378695000	-0.576156000
N	-2.458490000	4.287102000	-0.006617000
O	-3.440817000	3.790549000	0.564658000
O	-2.423836000	5.378707000	-0.576142000
2I			
I	3.113233000	-1.981463000	-0.013512000
I	-3.113235000	-1.981464000	-0.013510000
N	7.219862000	-0.622671000	0.014823000

N	-7.219861000	-0.622669000	0.014821000
C	6.069551000	-1.356703000	0.008736000
C	4.827134000	-0.748256000	0.002538000
C	4.721284000	0.678608000	0.004321000
C	5.951948000	1.399342000	0.012097000
C	7.160352000	0.744662000	0.017595000
C	3.499001000	1.351010000	-0.002811000
C	2.451417000	1.989137000	-0.006955000
C	1.230213000	2.677303000	-0.009215000
C	1.204450000	4.087468000	-0.009408000
C	-0.000001000	4.816403000	-0.008118000
C	-1.204452000	4.087466000	-0.009409000
C	0.000001000	1.929220000	-0.009075000
C	-1.230212000	2.677301000	-0.009216000
C	-2.451414000	1.989133000	-0.006956000
C	-3.498999000	1.351008000	-0.002812000
C	-4.721282000	0.678607000	0.004320000
C	-5.951945000	1.399342000	0.012093000
C	-7.160350000	0.744664000	0.017591000
C	-4.827134000	-0.748257000	0.002538000
C	-6.069551000	-1.356702000	0.008735000
C	8.544226000	-1.299673000	0.059153000
C	-8.544225000	-1.299672000	0.059155000
H	6.188489000	-2.435163000	0.008408000
H	5.937367000	2.485118000	0.011697000
H	8.111282000	1.268335000	0.024196000
H	2.154974000	4.616847000	-0.005082000
H	-2.154977000	4.616843000	-0.005085000
H	-5.937364000	2.485118000	0.011692000
H	-8.111279000	1.268338000	0.024190000
H	-6.188491000	-2.435162000	0.008409000
H	8.962781000	-1.214384000	1.067824000
H	9.212632000	-0.824413000	-0.664153000
H	8.415672000	-2.352228000	-0.200180000
H	-8.962758000	-1.214420000	1.067839000
H	-8.415678000	-2.352217000	-0.200222000
H	-9.212647000	-0.824384000	-0.664118000
N	0.000002000	0.577574000	-0.008903000
H	-0.873011000	0.059582000	-0.005938000
H	0.873016000	0.059583000	-0.005937000
N	-0.000002000	6.194998000	0.049461000
H	-0.853337000	6.694314000	-0.171089000

H 0.853329000 6.694316000 -0.171098000

2m

I -3.291031000 -2.343482000 -0.002109000
I 3.291032000 -2.343483000 -0.002106000
N -7.334359000 -0.807345000 -0.003890000
N 7.334359000 -0.807344000 -0.003892000
C -6.221004000 -1.592051000 -0.002143000
C -4.949777000 -1.039174000 -0.000558000
C -4.787077000 0.378991000 0.000250000
C -5.979506000 1.155813000 -0.000747000
C -7.217304000 0.554168000 -0.002676000
C -3.533579000 1.000848000 0.000323000
C -2.466870000 1.601447000 0.000182000
C -1.237080000 2.282038000 0.000119000
C -1.213526000 3.690044000 -0.000092000
C 0.000000000 4.368462000 -0.000197000
C 1.213525000 3.690043000 -0.000092000
C -0.000001000 1.541527000 0.000252000
C 1.237079000 2.282038000 0.000118000
C 2.466869000 1.601446000 0.000182000
C 3.533578000 1.000848000 0.000323000
C 4.787076000 0.378991000 0.000249000
C 5.979505000 1.155813000 -0.000749000
C 7.217303000 0.554169000 -0.002678000
C 4.949777000 -1.039174000 -0.000558000
C 6.221004000 -1.592051000 -0.002143000
C -8.691385000 -1.423407000 0.018721000
C 8.691386000 -1.423405000 0.018718000
H -6.387987000 -2.664165000 -0.002421000
H -5.916089000 2.239996000 -0.001689000
H -8.144556000 1.119041000 -0.003308000
H -2.140652000 4.255318000 -0.000182000
H 2.140652000 4.255317000 -0.000183000
H 5.916088000 2.239996000 -0.001691000
H 8.144555000 1.119042000 -0.003312000
H 6.387988000 -2.664164000 -0.002420000
H -8.598010000 -2.497322000 -0.151587000
H -9.298631000 -0.976640000 -0.773681000
H -9.153176000 -1.240401000 0.994536000
H 8.598010000 -2.497322000 -0.151581000
H 9.153181000 -1.240391000 0.994530000

H	9.298628000	-0.976643000	-0.773690000
N	-0.000001000	0.193944000	0.000541000
H	0.873140000	-0.324643000	0.000544000
H	-0.873142000	-0.324643000	0.000545000
N	0.000000000	5.860832000	-0.000427000
O	-1.102620000	6.421354000	-0.000512000
O	1.102622000	6.421353000	-0.000512000