Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

Exploiting Directional Long Range Secondary Forces for Regulating Electrostatics Dominated Noncovalent Interactions

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Table S1. Electrostatic Forces along the lines making angles 0°, 30°, 60°, 90°, up to 360° from the line connecting center of geometries of frontier atoms of hydrogen bonding partners for a sample set of 16 representative complexes of the planar hydrogen bond family

		0°	30°	60°	90°	120°	150°	180°	210°	240°	270°	300°	330°	360°
X-1	a	-163.4	-122.2	-48.3	38.6	115.1	160.8	163.4	122.2	48.3	-38.6	-115.1	-160.8	-163.4
	b	-451.8	-354.8	-162.8	72.9	289.0	427.7	451.8	354.8	162.8	-72.9	-289.0	-427.7	-451.8
	c	-101.3	-77.8	-33.5	19.8	67.8	97.6	101.3	77.8	33.5	-19.8	-67.8	-97.6	-101.3
X-2	a	-280.2	-207.8	-79.8	69.6	200.4	277.5	280.2	207.8	79.8	-69.6	-200.4	-277.5	-280.2
	b	-634.9	-524.8	-274.2	49.9	360.7	574.8	634.9	524.8	274.2	-49.9	-360.7	-574.8	-634.9
	c	-152.7	-120.1	-55.3	24.3	97.4	144.4	152.7	120.1	55.3	-24.3	-97.4	-144.4	-152.7
X-3	a	-253.6	-190.0	-75.6	59.1	178.0	249.1	253.6	190.0	75.6	-59.1	-178.0	-249.1	-253.6
	b	-541.1	-436.2	-241.5	17.9	272.5	454.1	514.1	436.2	241.5	-17.9	-272.5	-454.1	-514.1
	c	-133.8	-106.6	-51.1	18.2	82.7	125.0	133.8	106.6	51.1	-18.2	-82.7	-125.0	-133.8
X-4	a	-135.1	-96.6	-32.3	40.7	102.8	137.4	135.1	96.6	32.3	-40.7	-102.8	-137.4	-135.1
	b	-609.9	-447.7	-165.6	160.9	444.3	608.7	609.9	447.7	165.6	-160.9	-444.3	-608.7	-609.9
	c	-81.8	-59.7	-21.6	22.3	60.2	82.0	81.8	59.7	21.6	-22.3	-60.2	-82.0	-81.8
X-5	a	-326.4	-242.7	-93.9	80.0	232.5	322.7	326.4	242.7	93.9	-80.0	-232.5	-322.7	-326.4
	b	-667.5	-562.9	-307.6	30.2	359.9	593.1	667.5	562.9	307.6	-30.2	-359.9	-593.1	-667.5
	c	-161.8	-130.8	-64.8	18.6	97.1	149.5	161.8	130.8	64.8	-18.6	-97.1	-149.5	-161.8
X-6	a	-202.8	-148.4	-54.3	54.4	148.5	202.8	202.8	148.4	54.3	-54.4	-148.5	-202.8	-202.8
	b	-487.3	-409.9	-222.7	24.3	264.7	434.2	487.3	409.9	222.7	-24.3	-264.7	-434.2	-487.3
	c	-117.0	-93.1	-44.2	16.5	72.8	109.6	117.0	93.1	44.2	-16.5	-72.8	-109.6	-117.0
X-7	a	-267.0	-195.1	-71.0	72.2	196.0	267.3	267.0	195.1	71.0	-72.2	-196.0	-267.3	-267.0
	b	-568.4	-484.9	-271.5	14.7	296.9	499.6	568.4	484.9	271.5	-14.7	-296.9	-499.6	-568.4
	c	-151.3	-120.1	-56.7	21.9	94.7	142.0	151.3	120.1	56.7	-21.9	-94.7	-142.0	-151.3
X-8	a	-450.8	-333.7	-127.2	113.4	323.6	447.1	450.8	333.7	127.2	-113.4	-323.6	-447.1	-450.8
	b	-812.1	-680.5	-366.6	45.6	445.5	726.1	812.1	680.5	366.6	-45.6	-445.5	-726.1	-812.1
	c	-245.9	-193.6	-89.3	38.8	156.6	232.4	245.9	193.6	89.3	-38.8	-156.6	-232.4	-245.9
X-9	a	-75.8	-51.6	-13.5	28.2	62.3	79.7	75.8	51.6	13.5	-28.2	-62.3	-79.7	-75.8
	b	-321.0	-256.2	-122.7	43.7	198.3	299.8	321.0	256.2	122.7	-43.7	-198.3	-299.8	-321.0
	c	-66.1	-51.1	-22.4	12.3	43.7	63.4	66.1	51.1	22.4	-12.3	-43.7	-63.4	-66.1
X-10	a	-95.5	-58.4	-5.7	48.5	89.8	107.0	95.5	58.4	5.7	-48.5	-89.8	-107.0	-95.5
	b	-307.7	-262.0	-146.1	9.0	161.7	271.0	307.7	262.0	146.1	-9.0	-161.7	-271.0	-307.7
	c	-89.3	-70.7	-33.1	13.3	56.2	84.0	89.3	70.7	33.1	-13.3	-56.2	-84.0	-89.3
X-11	a	-521.1	-399.3	-170.6	103.9	350.5	503.2	521.1	399.3	170.6	-103.9	-350.5	-503.2	-521.1
	b	-1173.3	-931.5	-440.1	169.2	733.2	1100.7	1173.3	931.5	440.1	-169.2	-733.2	-1100.7	-1173.3
	c	-241.0	-190.4	-88.7	36.7	152.3	227.1	241.0	190.4	88.7	-36.7	-152.3	-227.1	-241.0
X-12	a	-273.3	-212.8	-96.2	46.1	176.0	258.8	272.3	212.8	96.2	-46.1	-176.0	-258.8	-273.3
	b	-869.5	-684.0	-315.2	138.1	554.3	822.0	869.5	684.0	315.2	-138.1	-554.3	-822.0	-869.5
	c	-163.2	-129.9	-61.8	22.9	101.4	152.8	163.2	129.9	61.8	-22.9	-101.4	-152.8	-163.2
X-13	a	-301.8	-208.6	-59.5	105.5	242.2	314.1	301.8	208.6	59.5	-105.5	-242.2	-314.1	-301.8
	b	-674.3	-455.8	-115.1	256.4	559.2	712.2	674.3	455.8	115.1	-256.4	-559.2	-712.2	-674.3
	c	-160.0	-107.8	-26.8	61.5	133.2	169.3	160.0	107.8	26.8	-61.5	-133.2	-169.3	-160.0
X-14	a	-167.9	-135.3	-66.4	20.3	101.6	155.6	167.9	135.3	66.4	-20.3	-101.6	-155.6	-167.9
	b	-680.4	-547.3	-267.6	83.9	412.8	631.2	680.4	547.3	267.6	-83.9	-412.8	-631.2	-680.4
	c	-164.7	-139.6	-77.0	6.1	87.7	145.7	164.7	139.6	77.0	-6.1	-87.7	-145.7	-164.7
X-15	a	-243.8	-185.2	-77.0	51.8	166.8	237.0	243.8	185.2	77.0	-51.8	-166.8	-237.0	-243.8
	b	-846.0	-670.8	-315.8	123.8	530.3	794.6	846.0	670.8	315.8	-123.8	-530.3	-794.6	-846.0
	c	-166.2	-126.8	-53.4	34.3	112.8	161.1	166.2	126.8	53.4	-34.3	-112.8	-161.1	-166.2
X-	a	-105.0	-74.5	-24.0	32.9	81.0	107.4	105.0	74.5	24.0	-32.9	-81.0	-107.4	-105.0

16	b	-621.9	-459.1	-173.4	158.9	448.5	618.0	621.9	459.1	173.4	-158.9	-448.5	-618.0	-621.9
	c	-108.0	-78.5	-28.1	29.9	79.9	108.5	108.0	78.5	28.1	-29.9	-79.9	-108.5	-108.0

a = computed electrostatic force using Mulliken Charges; b = computed electrostatic force using NBO Charges; c = computed electrostatic force using Lowdin Charges; All forces are in pN; Please see the Figure S3 below for the optimized geometry of X-1 to X-16.

Table S2. Binding Energies and Electrostatic Forces for planar hydrogen bonded complexes optimized at the COSMO ($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4.

Planar hydrogen bonded complex	Binding Energy	EF (with Mulliken Charges analysis)	EF (with NBO Charges analysis)
X-1	-15.4	-163.4	-451.8
X-2	-29.2	-280.2	-634.9
X-3	-19.3	-253.6	-514.1
X-4	-14.9	-135.1	-609.9
X-5	-29.4	-326.4	-667.5
X-6	-18.0	-202.8	-487.3
X-7	-22.3	-267.0	-568.4
X-8	-42.9	-450.8	-812.1
X-9	-14.3	-75.8	-321.0
X-10	-17.3	-167.6	-307.7
X-11	-43.4	-521.1	-1173.3
X-12	-26.4	-272.3	-869.5
X-13	-33.9	-301.8	-674.3
X-14	-20.7	-167.9	-680.4
X-15	-30.9	-243.8	-846.0
X-16	-20.6	-105.0	-621.9

EF=Electrostatic Force

All forces are in pN

All energies are in kcal/mol.

Please see the Figure S3 below for the optimized geometry of X-1 to X-16.

Table S3. Binding Energies and Electrostatic Forces for planar hydrogen bonded complexes optimized at the CPCM($CHCl_3$)/M06-2X/6-31G level of theory using Gaussian 09.**

Planar hydrogen bonded complex	Binding Energy	EF (with Mulliken Charges analysis)	EF (with NBO Charges analysis)
Y-1	-15.8	-183.1	-468.1
Y-2	-28.3	-418.3	-689.8
Y-3	-19.3	-154.1	-242.4
Y-4	-16.0	-338.4	-489.7
Y-5	-28.3	-360.3	-648.5
Y-6	-20.0	-272.8	-526.9
Y-7	-23.6	-297.2	-415.1
Y-8	-17.3	-125.8	-391.4
Y-9	-41.1	-801.4	-1283.8
Y-10	-28.3	-446.1	-889.2
Y-11	-28.3	-575.7	-635.0
Y-12	-30.2	-555.2	-1021.6
Y-13	-18.7	-315.1	-613.8
Y-14	-28.0	-598.4	-1111.4
Y-15	-20.3	-387.9	-699.0
Y-16	-18.0	-165.7	-614.4

EF=Electrostatic Force

All forces are in pN

All energies are in kcal/mol.

Please see Figure S4 below for the optimized geometries of Y-1 to Y-16.

Table S4. Binding Energy, Interaction Energy and Electrostatic Forces for Nitrogenous Base Complexes optimized at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4.

Molecule Name	Binding Energy	Interaction Energy	EF (with Mulliken Charges analysis)	EF (with NBO Charges analysis)
AA1	-11.8	-13.1	-297.2	-275.5
AA2	-11.3	-12.5	-154.5	-451.8
AA3	-10.0	-11.0	-17.2	-471.1
AC1	-13.0	-14.4	-360.2	-448.8
AC2	-12.7	-14.0	-230.4	-608.4
AT (H)	-11.6	-14.4	-270.3	-772.0
AT (RH)	-12.5	-14.0	-289.9	-733.8
AT (RWC)	-11.1	-14.1	-330.7	-520.0
AT (WC)	-12.7	-14.6	-408.8	-554.5
CC	-14.9	-16.6	-409.0	-607.4
GA1	-14.0	-15.7	-381.3	-702.2
GA2	-10.1	-11.4	-146.9	-424.6
GA3	-13.4	-15.0	-244.7	-716.4
GA4	-11.2	-12.6	-266.1	-340.7
GC	-21.5	-23.8	-577.0	-1110.0
GC1	-12.0	-12.7	-316.7	-823.1
GC2	-12.6	-14.1	-335.2	-374.4
GG1	-18.3	-20.7	-535.3	-1620.0
GG3	-15.2	-16.1	-304.3	-707.7
GG4	-9.7	-10.9	-227.2	-315.5
GT1	-13.2	-14.9	-412.7	-608.4
GT2	-11.1	-13.7	-343.8	-462.7
TC1	-9.6	-11.1	-272.6	-340.7
TC2	-8.9	-10.2	-239.0	-351.4
TT1	-8.7	-11.0	-309.1	-438.6
TT2	-10.4	-11.8	-343.1	-455.6
TT3	-8.2	-10.4	-255.8	-370.8
U-DAP	-14.6	-17.1	-440.1	-884.0

EF=Electrostatic Force

All forces are in pN

All energies are in kcal/mol.

Representation of molecular complexes has been taken from the Popelier's paper cited into the manuscript. The optimized geometries are provided into Figure S8 below.

Table S5. Binding Energies and Electrostatic Forces for contact ion-pairs at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4.

Anion	Binding Energy	EF (with Mulliken Charges analysis)	EF (with NBO Charges analysis)
Z-1	-35.1	-300.5	-400.0
Z-2	-35.2	-215.1	-242.4
Z-3	-56.9	-393.4	-510.8
Z-4	-51.3	-288.3	-332.2
Z-8	-56.8	-500.9	-975.2
Z-6	-34	-220.0	-268.7
Z-4	-30.8	-140.4	-201.0
Z-5	-30.7	-94.1	-185.7

EF=Electrostatic Force

All forces are in pN

All energies are in kcal/mol.

Please see the Figure S5 below for the optimized geometries of **Z-1** to **Z-8**.

Table S6. Binding Energies and Electrostatic Forces for hypothetical newly designed cationic AAAA-DDDD complexes obtained at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4.

Designed planar AAAA-DDDD cationic complex	Binding Energy	EF (with Mulliken Charges analysis)	EF (with NBO Charges analysis)
A-1	-49.6	-675.119	-1501.921
A-2	-49.2	-802.126	-1535.602
A-3	-55.7	-828.445	-1868.424
A-4	-60.2	-1264.118	-2202.395
B-1	-50.2	-641.838	-1313.852
B-2	-50.8	-524.964	-1127.156
C	-69.6	-1411.299	-2795.471

EF=Electrostatic Force

All forces are in pN

All energies are in kcal/mol.

Please refer Figures S9, S11 and S12 below to see the optimized geometries **A-1** to **C**.

Table S7. Binding Energies for hypothetical newly designed planer hydrogen bonded complexes obtained at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4.

Designed planar AAAA-DDDD cationic complex	Binding Energy	ΔE [a]
D-1	-17.3	1.9
D-2	-37.2	8.0
D-3	-23.8	4.5
D-4	-45.2	11.3

a= increase in binding strength, which was compared with respect to the corresponding synthesized parental complexes wherefrom they are derived.

All energies are in kcal/mol.

Please refer Figure S13 below to for the structures of **D-1** to **D-4**.

Table S8. Binding Energies for hypothetical newly designed planer hydrogen bonded complexes obtained at the COSMO/PBE/TZVP level of theory using Turbomole 6.4.

Designed planar AAAA-DDDD cationic complex	Binding Energy	ΔE [a]
E-1	-47.3	3.9
E-2	-45.9	2.5
E-3	-46.4	3.0
E-4	-45.3	1.9

a= increase in binding strength, which was compared with respect to the corresponding synthesized parental complexes wherefrom they are derived.

All energies are in kcal/mol.

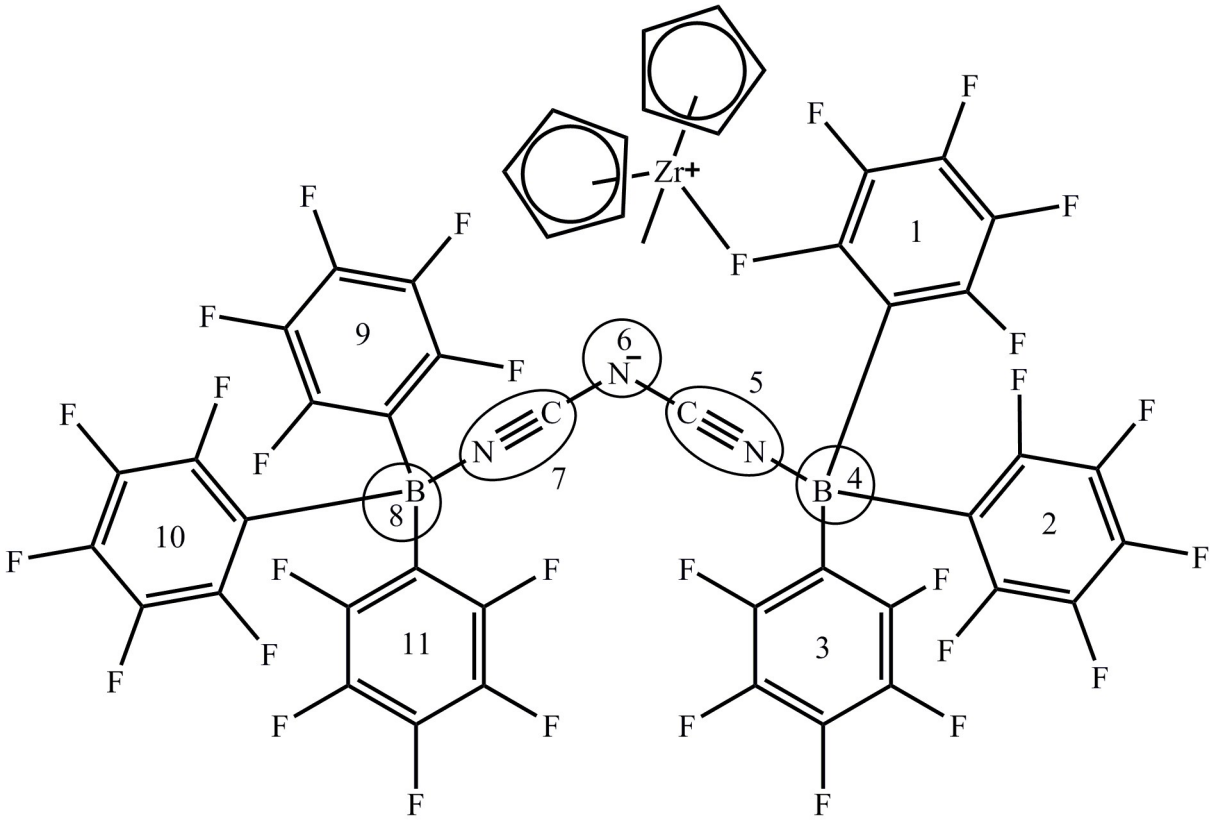
Please refer Figure S14 below for the structures of **E-1** to **E-4**.

Table S9. Electrostatic Forces analysis for zirconocne complex with best Bochmann's anion on Mulliken charge analysis for the geometry obtained at the COSMO/PBE/TZVP level of theory using Turbomole 6.4.

Region	1	2	3	4	5	6	7	8	9	10	11
Force	-90.5	-2.1	-9.6	22.6	38.4	-56.4	31.5	6.0	-6.9	-14.9	-12.2

All the Forces are in pN.

Please see the following attached structure to refer the corresponding regions of the molecule.



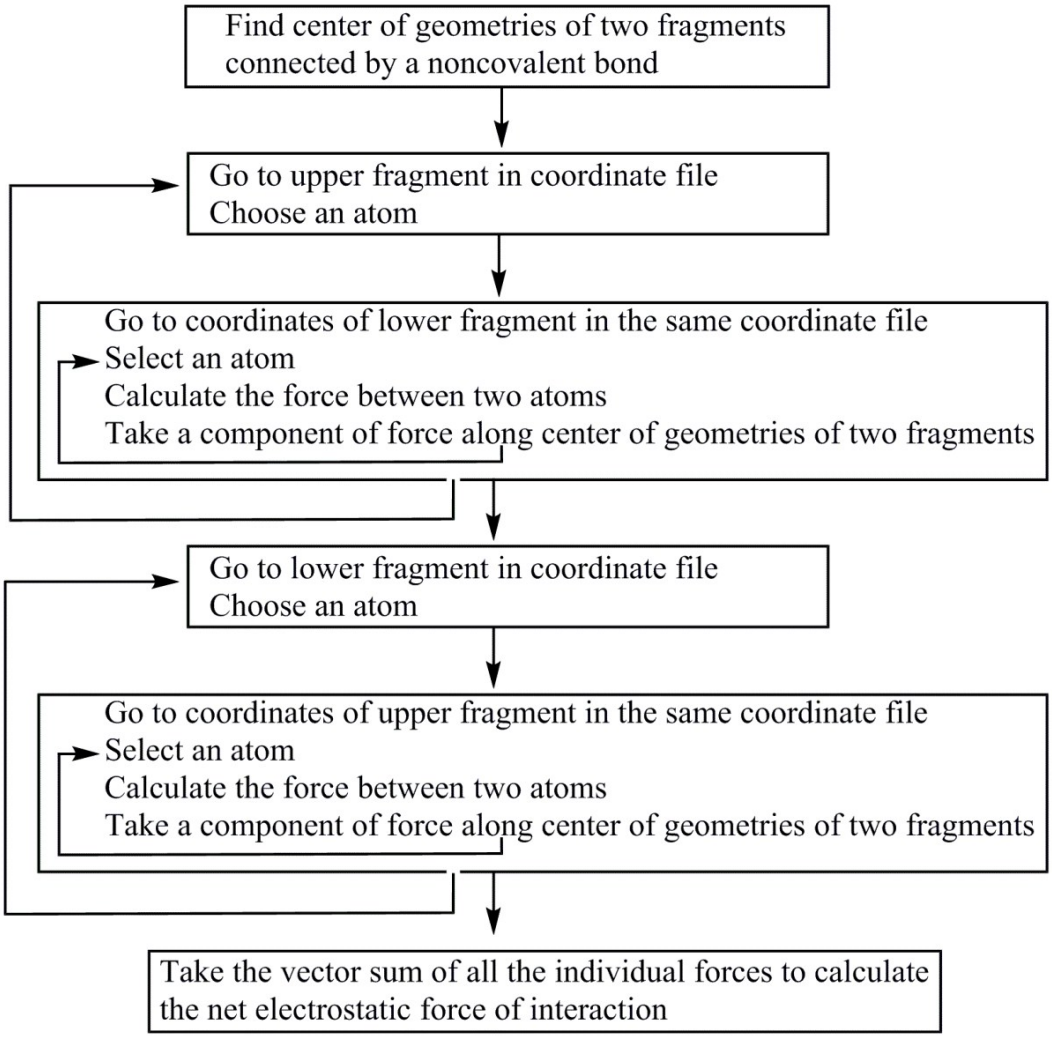


Figure S1. Flow chart of the Fortran 90 code used for calculating net force between two partners in hydrogen bonded complexes.

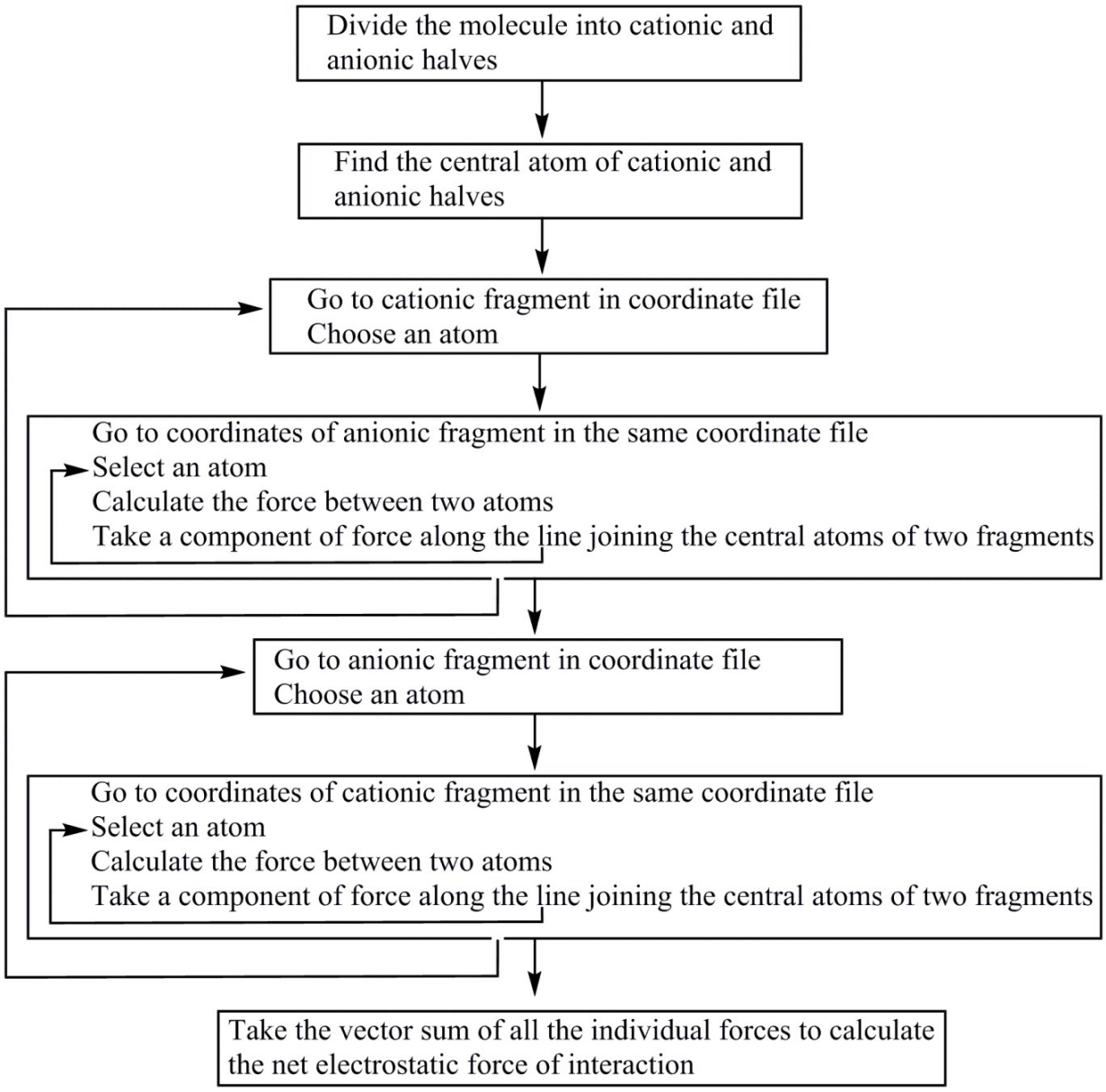
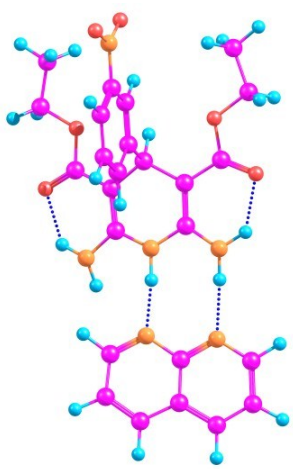
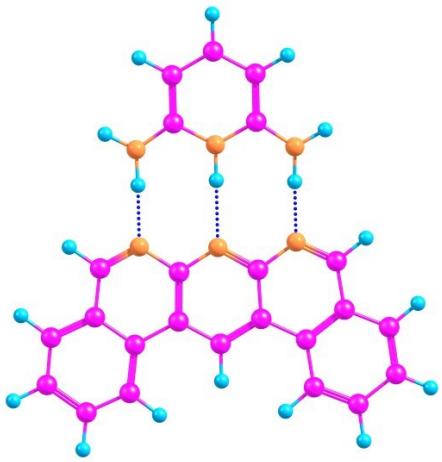


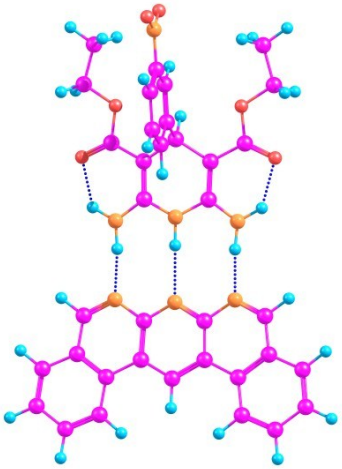
Figure S2. Flow chart of the Fortran 90 code used for calculating net force between two partners in Contact ion-pairs case.



X-1



X-2



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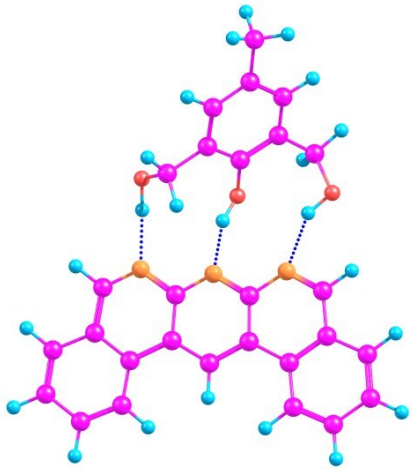

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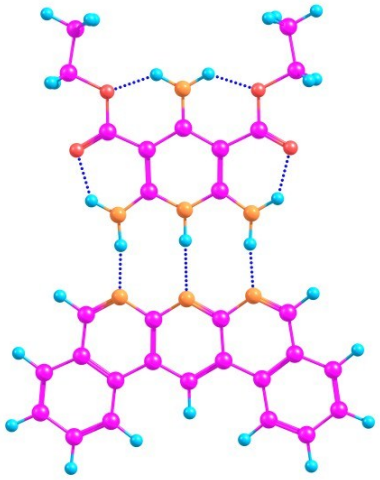

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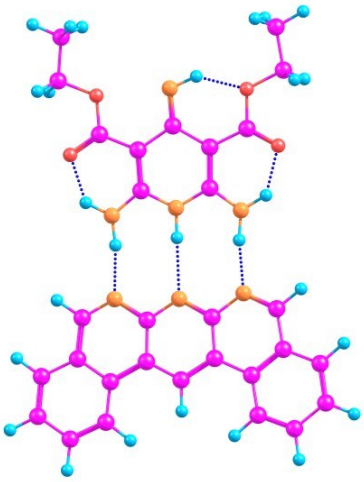

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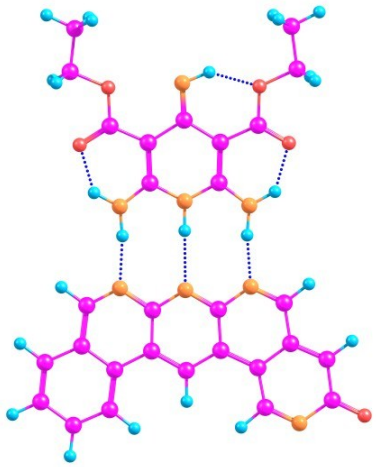

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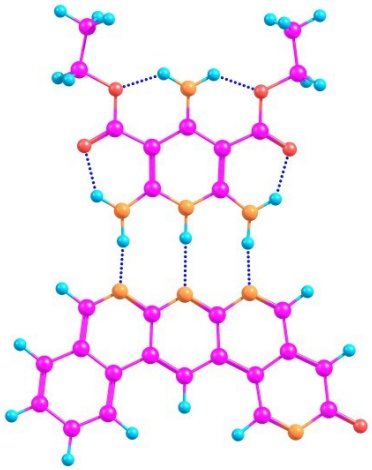

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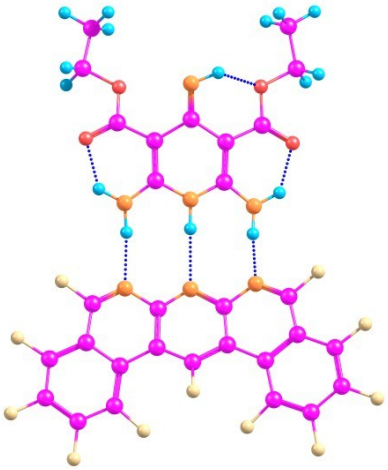

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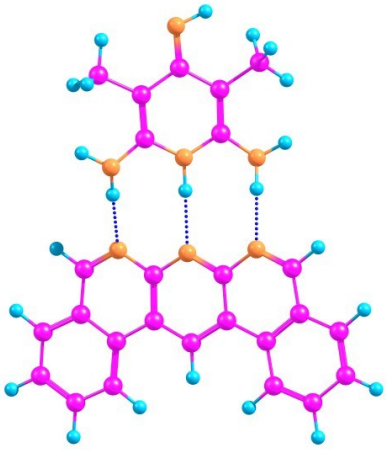
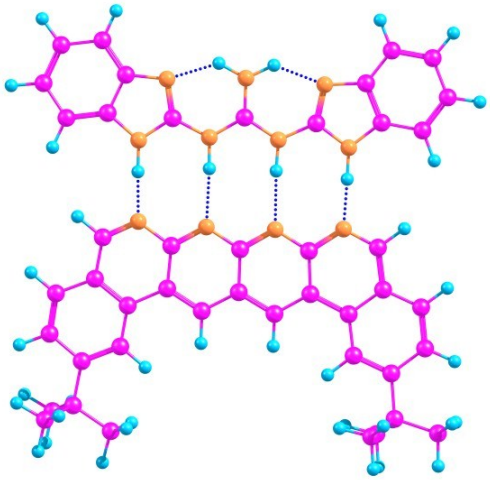
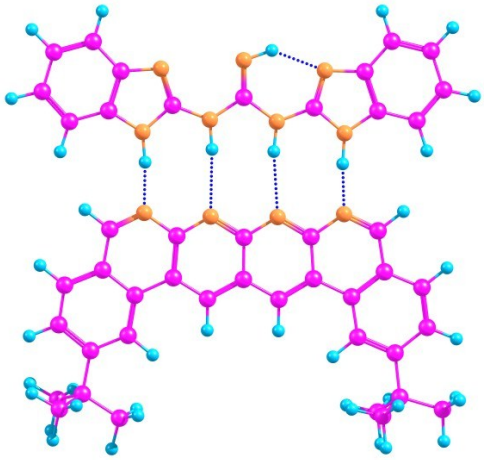


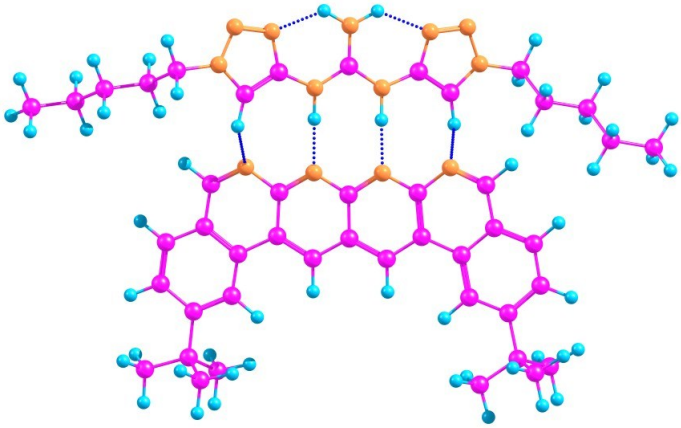
X-10



X-11

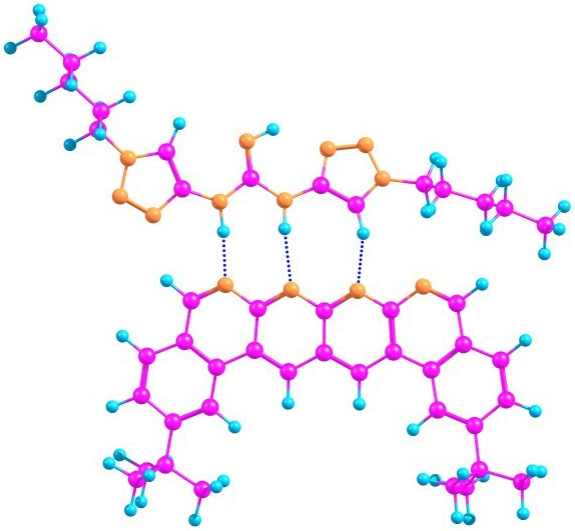


X-12

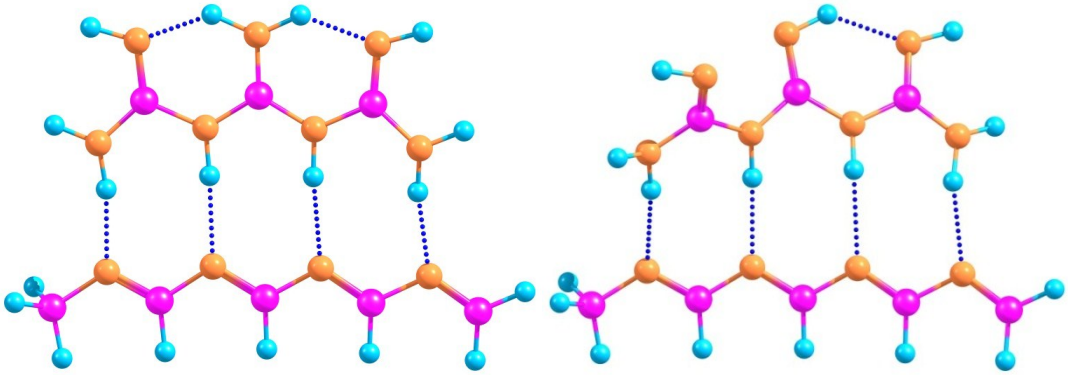


X-13

(Figure continued)

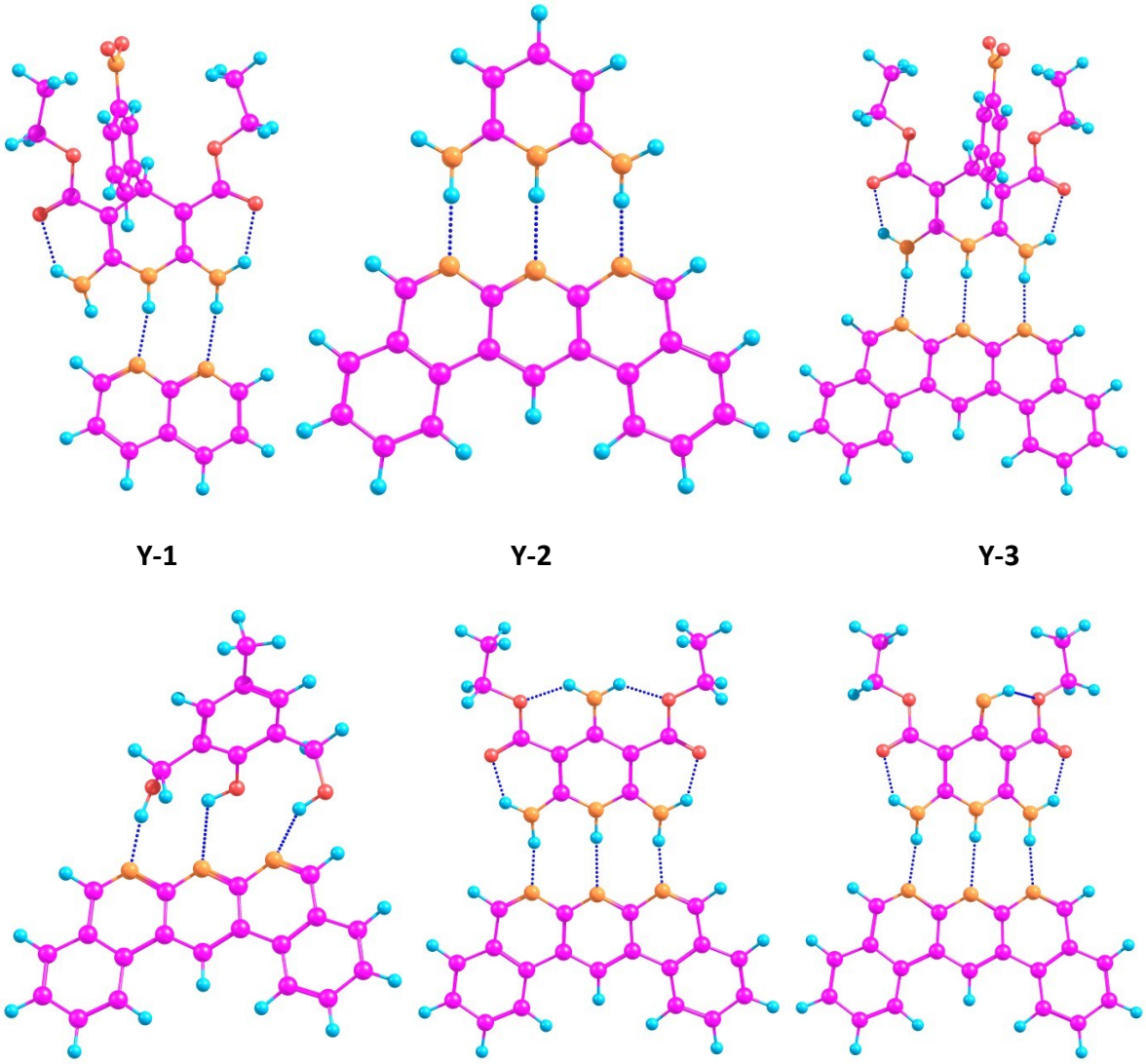


X-14



X-15 **X-16**

Figure S3. The optimized geometries of planar hydrogen bonded complexes at the COSMO($CHCl_3$)/PBE/TZVP level of theory. Pink, cyan, brown and white colors represent carbon, hydrogen, nitrogen and fluorine atoms respectively, whereas, dotted blue lines represent hydrogen bonds. **X-5** to **X-10, X-15** and **X-16** are optimized geometries of modeled complexes that are obtained after modification on non-frontier region of corresponding Leigh's complexes.



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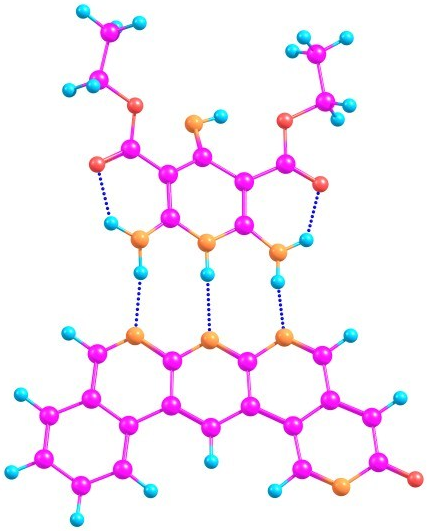
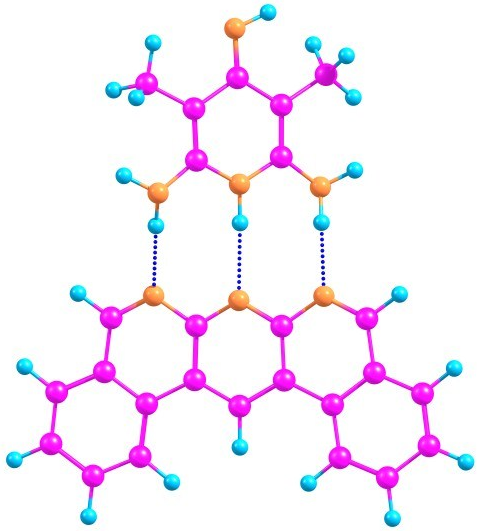
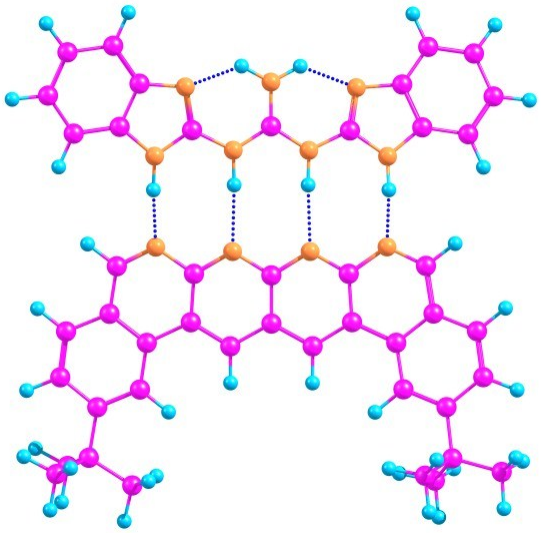


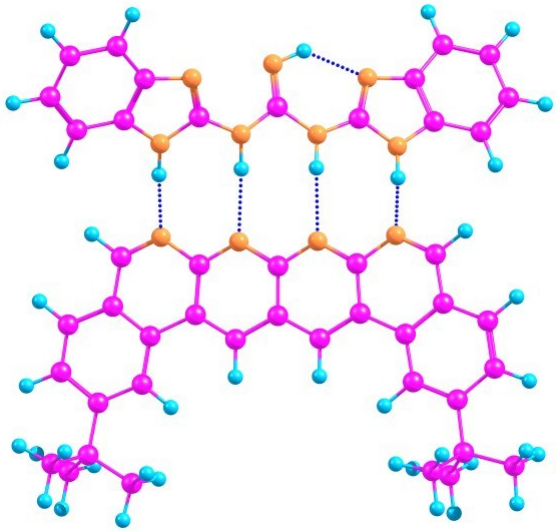
Y-7



Y-8



Y-9



Y-10

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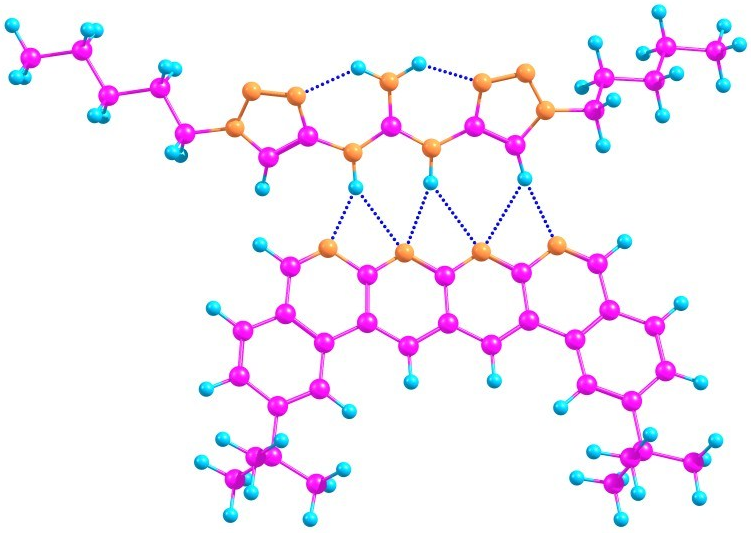
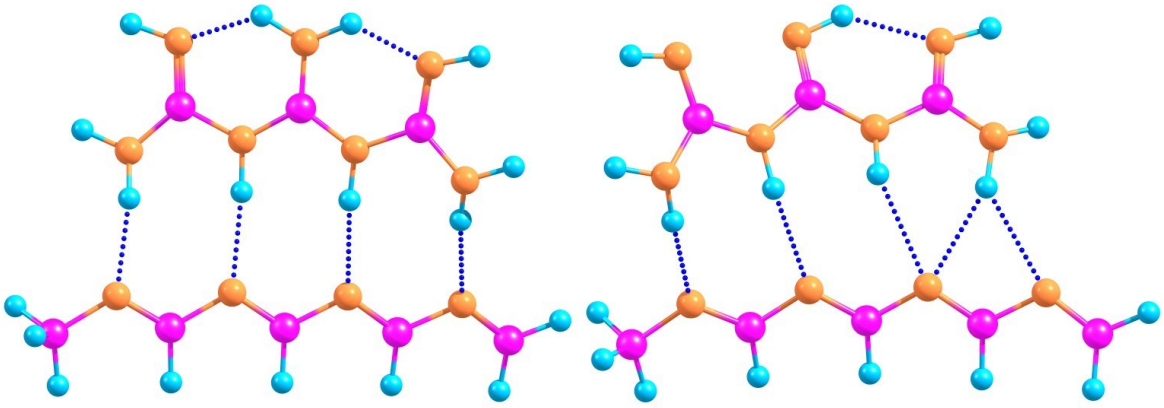
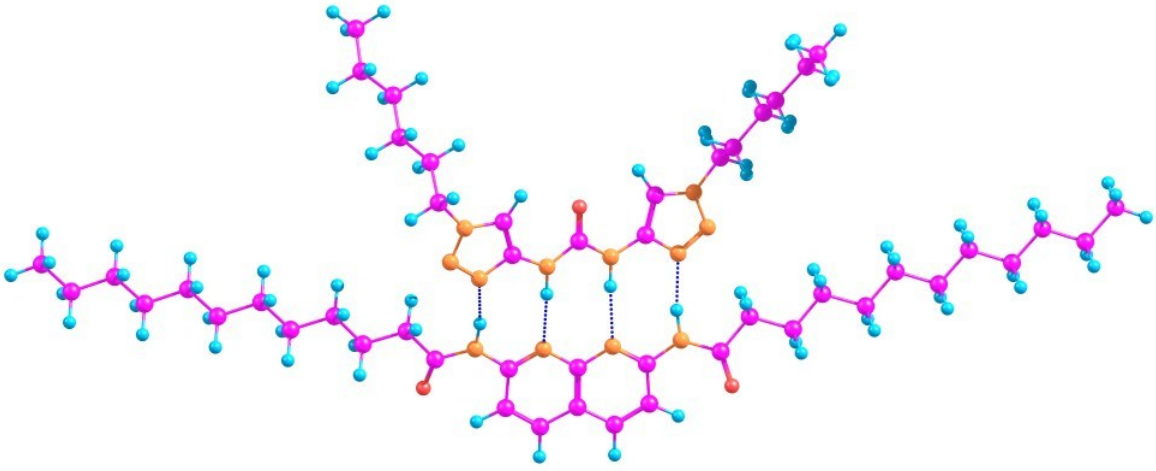


Y-11



Y-12 **Y-13**



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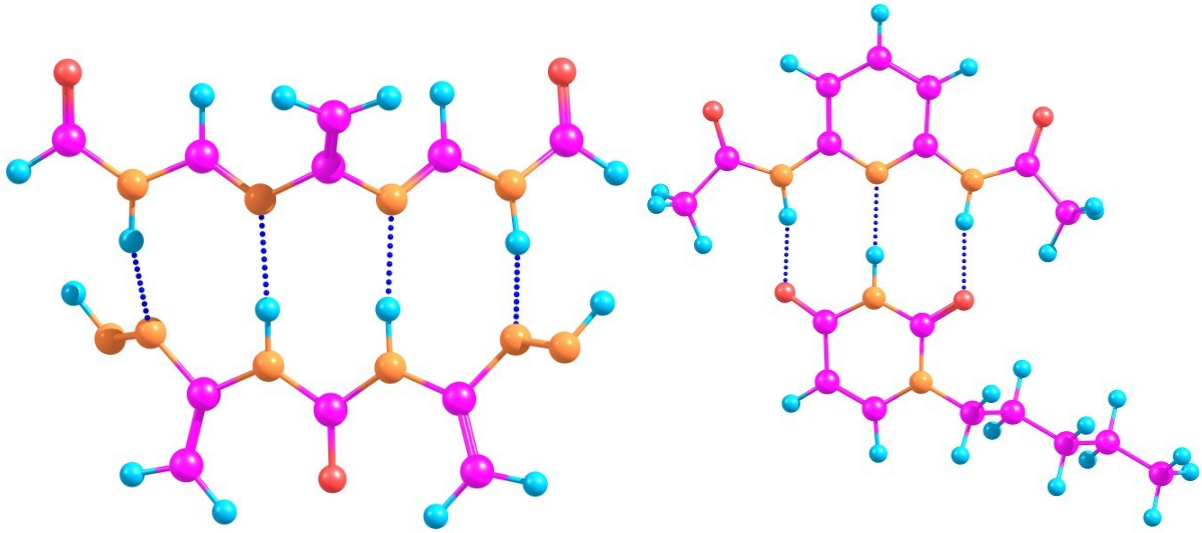
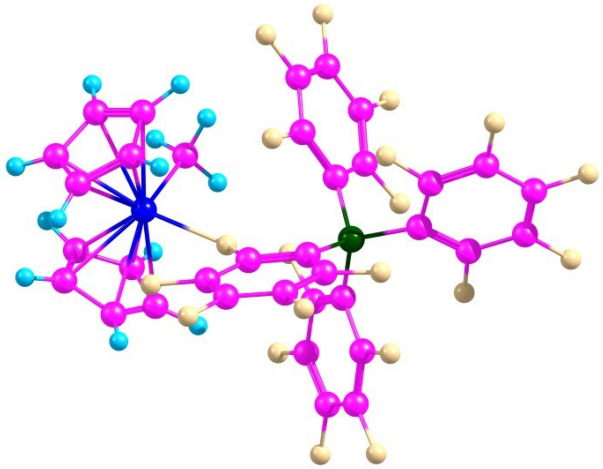


Y-15 **Y-16**

Figure S4. The optimized geometries of planar hydrogen bonded complexes at the CPCM($CHCl_3$)/M06-2X/6-31G** level of theory. Pink, cyan, brown and white colors represent carbon, hydrogen, nitrogen and fluorine atoms respectively, whereas, dotted blue lines represent hydrogen bonds. **Y-5** and **Y-12** to **Y-14** are optimized geometries of modeled complexes that are obtained after modification on non-frontier region of corresponding Leigh's or Yosuke complexes.



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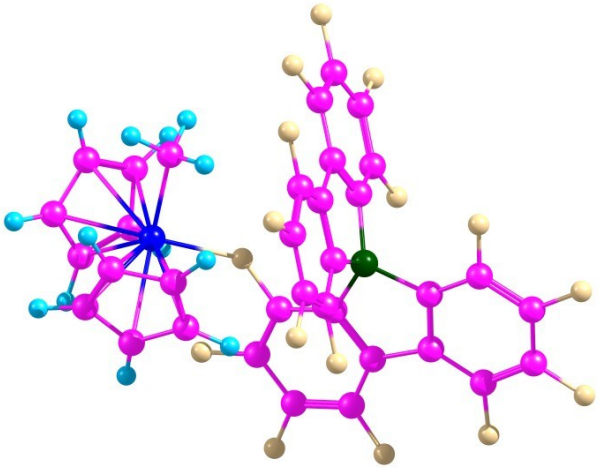
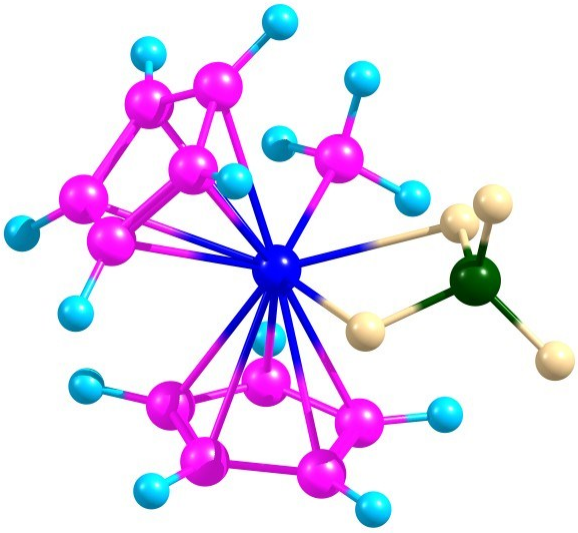
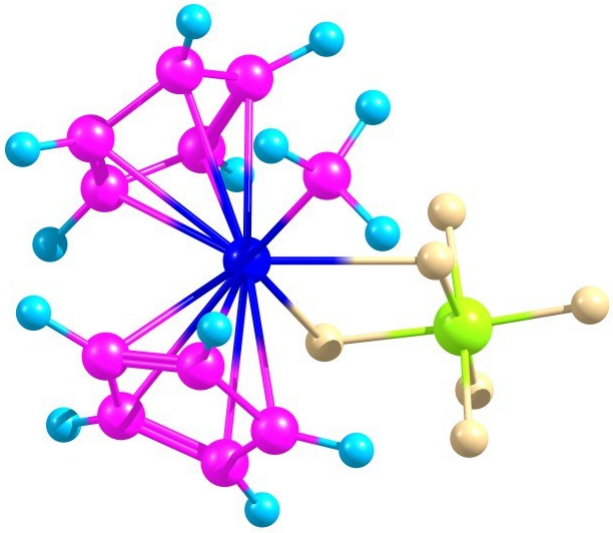


Z-2



Z-3



Z-4

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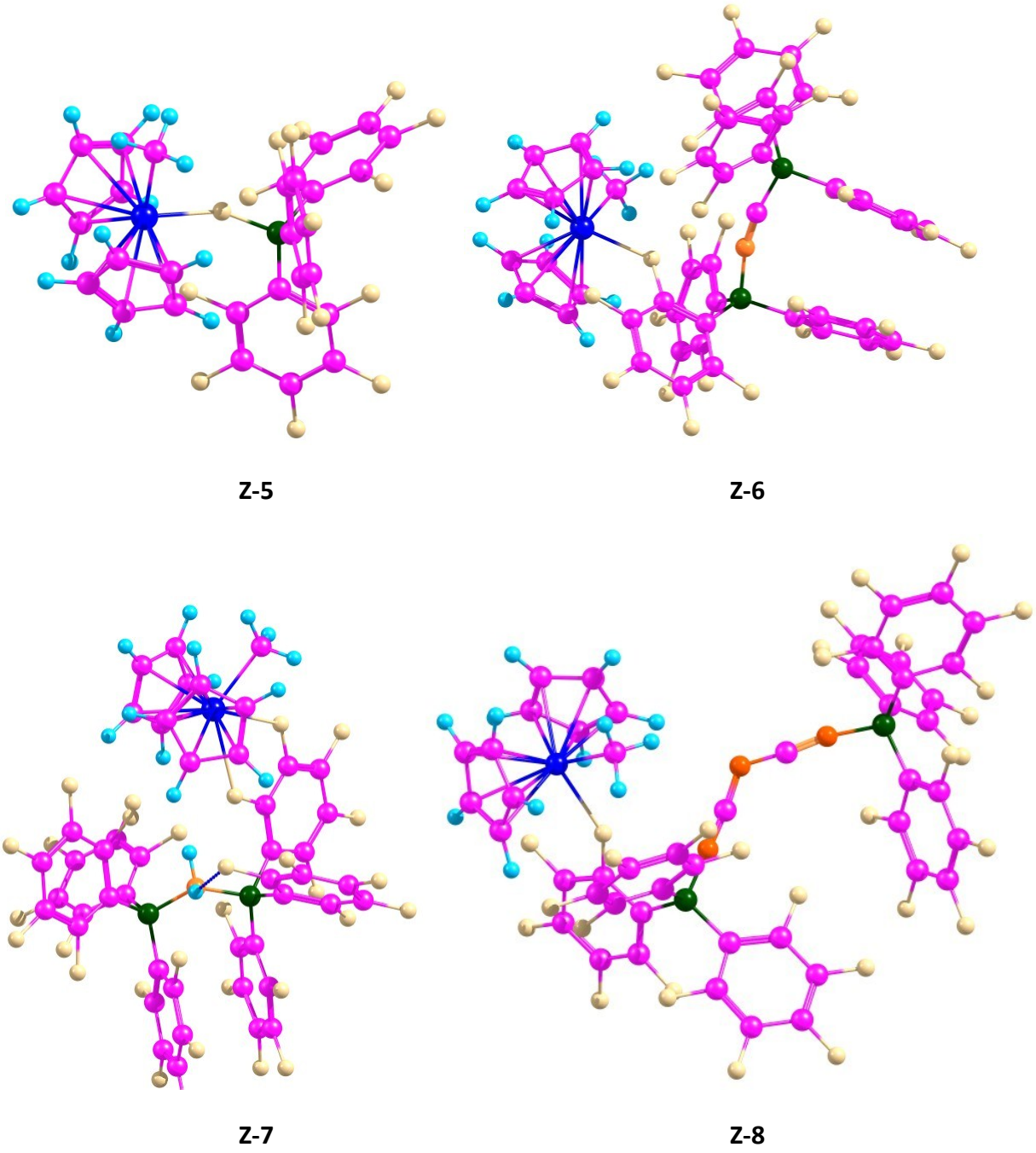


Figure S5. The optimized geometries of ion-pair complexes at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4. Pink, cyan, brown, green, blue, lime and white colors represent carbon, hydrogen, nitrogen, boron, zirconium, phosphorous and fluorine atoms respectively, whereas, dotted blue lines represent hydrogen bonds.

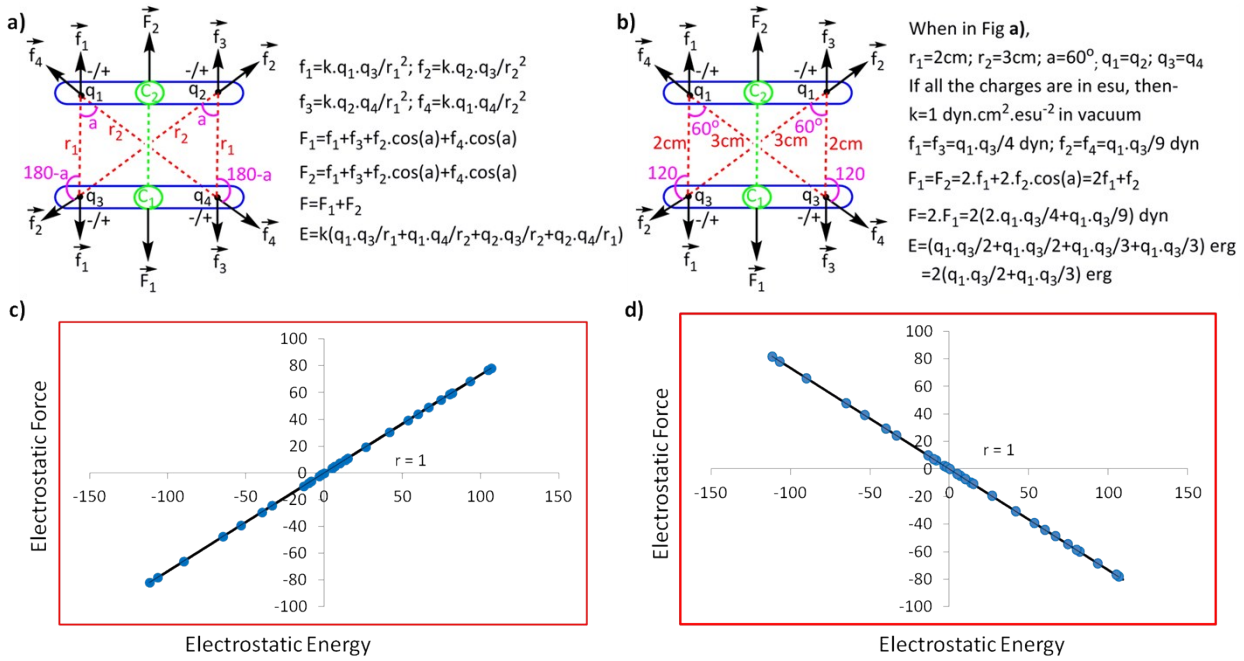


Figure S6. a) A simple model representing the electrostatic interaction between the two partners, each made up of two point charges of the same nature, in a two dimensional plane. f_1, f_2, f_3, f_4 represent the magnitude of forces experienced by the corresponding charged particles due to the charges on the other partner. C_1 and C_2 are the center of geometries of the two particles on the respective partners. The line joining C_1 and C_2 is the line of direction. F_1 and F_2 are the magnitude of forces experienced by the respective partners. F is the magnitude of the force of interaction between two partners. E is the electrostatic energy of interaction. b) A further simplified model when magnitude and nature of both the charges on each fragment are the same. c) The Pearson correlation graph between the electrostatic force of interaction along the direction of approach of the two partners and the electrostatic energy of interaction under the conditions described in b) for a set of 30 different values of q_1 and q_2. The forces are in dyn and the energies are in erg. d) The Pearson correlation graph between the electrostatic force of interaction along the direction opposite to the direction of approach of the two partners and the electrostatic energy of interaction under the conditions described in b) for the same set of 30 different values of q_1 and q_2.

The values of the force and the energies obtained for different values of q_1 and q_2 are provided below:

q1	q3	E	F (at 0°)	F (at 180°)
3	-18	-90.0	-66.0	66.0
2	-4	-13.3	-9.8	9.8
3	-13	-65.0	-47.7	47.66666667
4	4	26.66666667	19.55555556	-19.55555556
5	5	41.66666667	30.55555556	-30.55555556
6	6	60.0	44.0	-44.0
7	7	81.66666667	59.88888889	-59.88888889
8	8	106.6666667	78.22222222	-78.22222222
8	1	13.33333333	9.777777778	-9.777777778
8	-4	-53.33333333	-39.11111111	39.11111111
8	-3	-40.0	-29.33333333	29.33333333
8	4	53.33333333	39.11111111	-39.11111111
8	5	66.66666667	48.88888889	-48.88888889
8	6	80.0	58.66666667	-58.66666667
8	7	93.33333333	68.44444444	-68.44444444
8	-8	-106.6666667	-78.22222222	78.22222222
5	-1	-8.333333333	-6.111111111	6.111111111
-1	6	-10.0	-7.333333333	7.333333333
-1	-3	5.0	3.666666667	-3.666666667
-2	10	-33.33333333	-24.44444444	24.44444444
-2	-2	6.666666667	4.888888889	-4.888888889
-2	-3	10.00000000	7.333333333	-7.333333333
-3	-1	5.0	3.666666667	-3.666666667
-3	-2	10.0	7.333333333	-7.333333333
-3	-3	15.0	11.0	-11.0
1	-2	-3.333333333	-2.444444444	2.444444444
-1	1	-1.666666667	-1.222222222	1.222222222
0.2	0.1	0.033333333	0.024444444	-0.024444444
10.3	6.1	104.7166667	76.79222222	-76.79222222
5.2	8.6	74.53333333	54.65777778	-54.65777778
9.7	-6.9	-111.55	-81.80333333	81.80333333

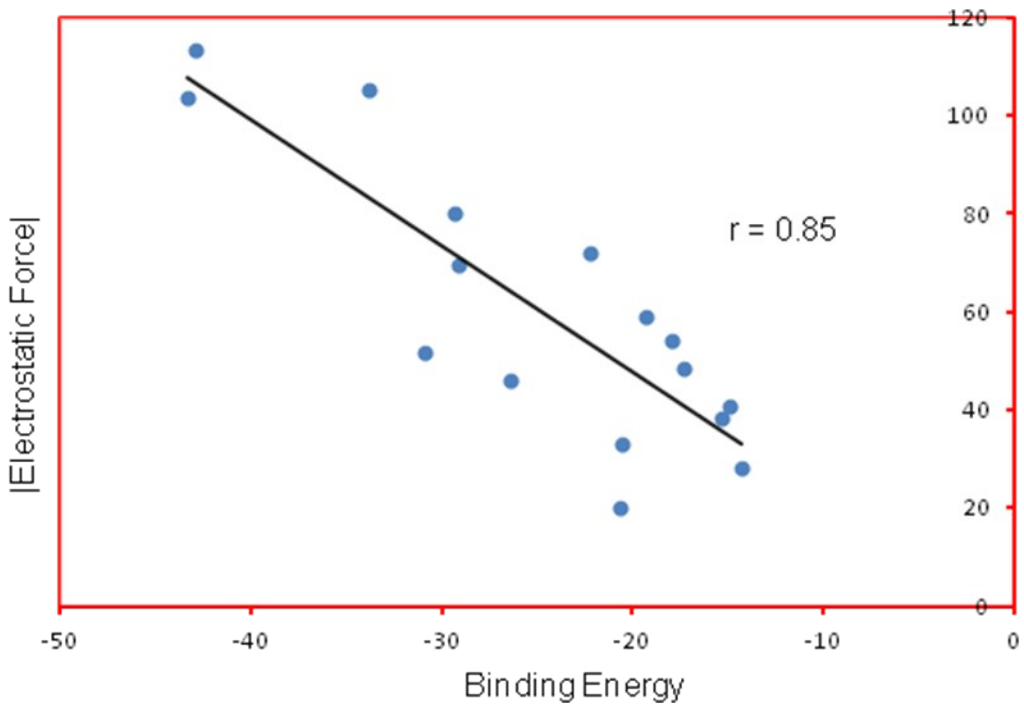
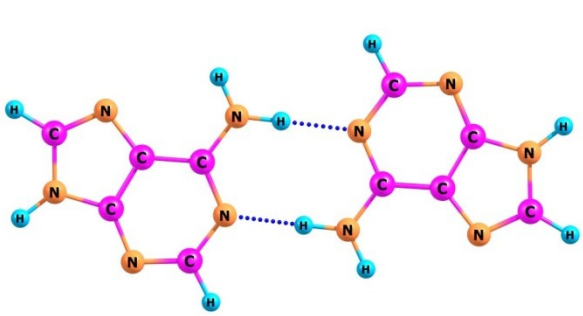


Figure S7. The EF vs. E_b Pearson Correlation graph for planar hydrogen bonded molecules for forces calculated along a line perpendicular to the line of direction of hydrogen bonds, by employing Mulliken charges for the geometries obtained at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4 package.



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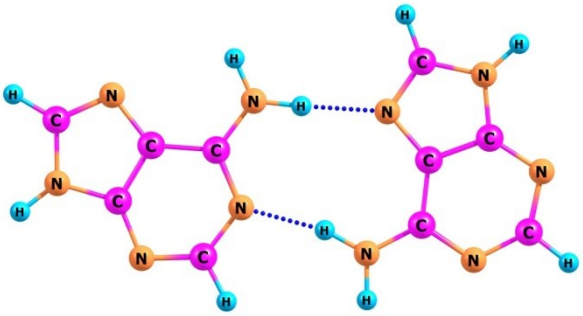

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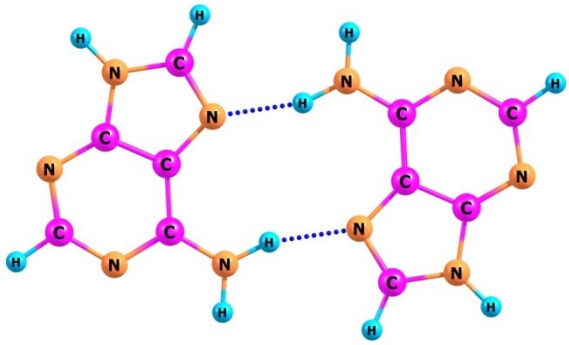

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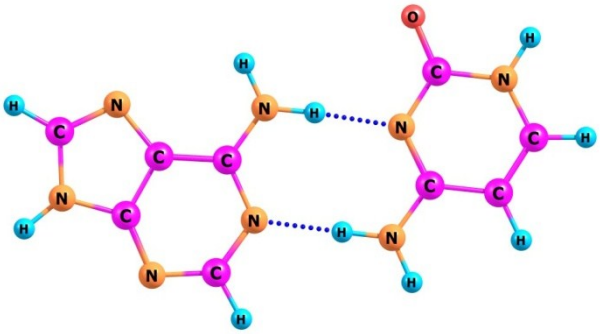

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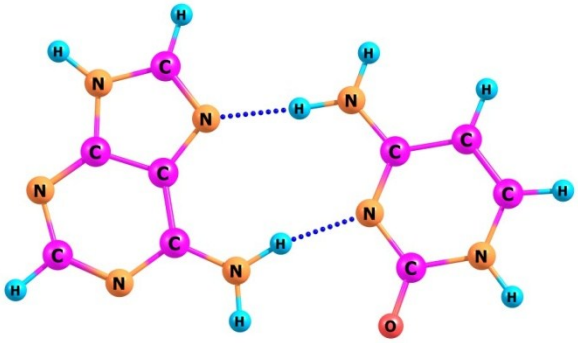

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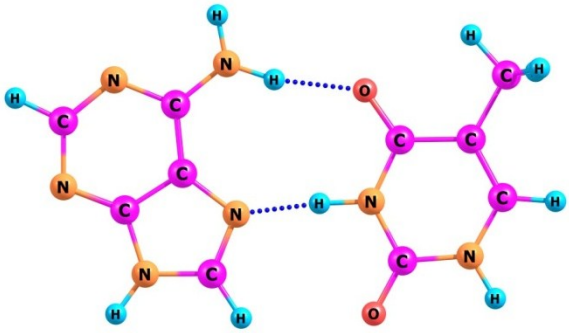

AT (H)

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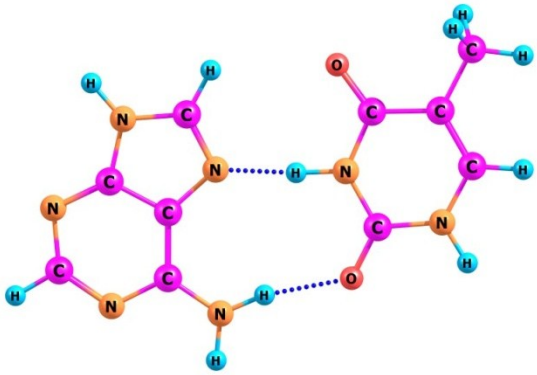

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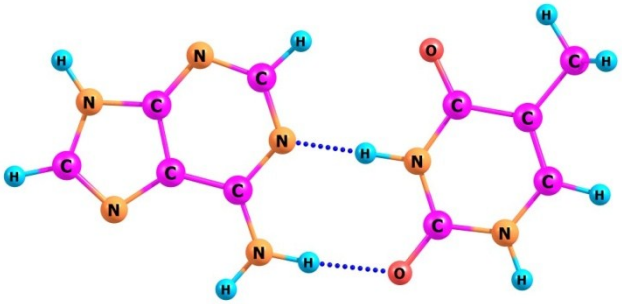

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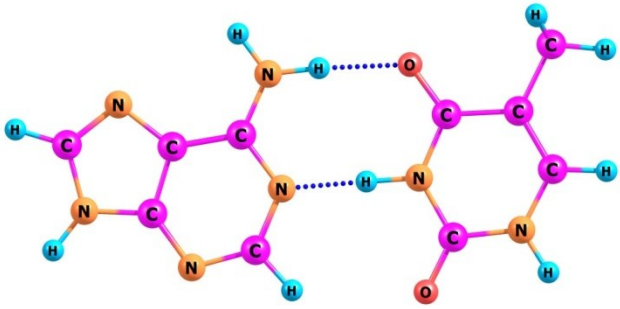

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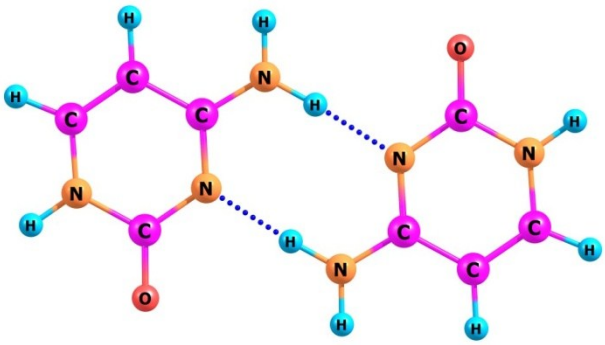

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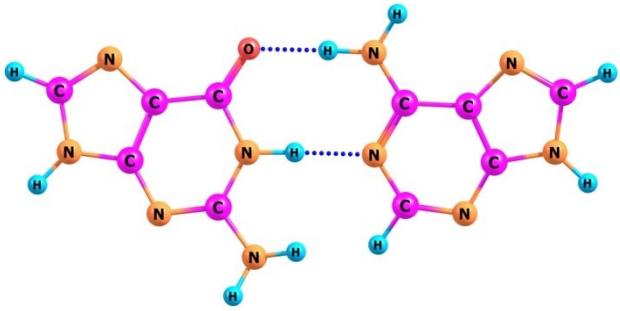

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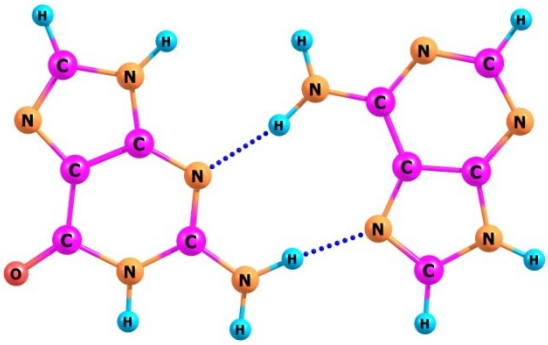

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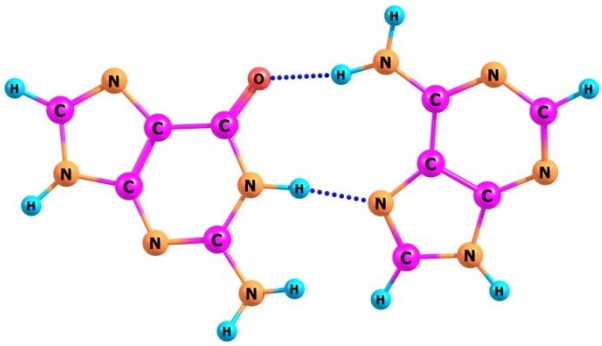

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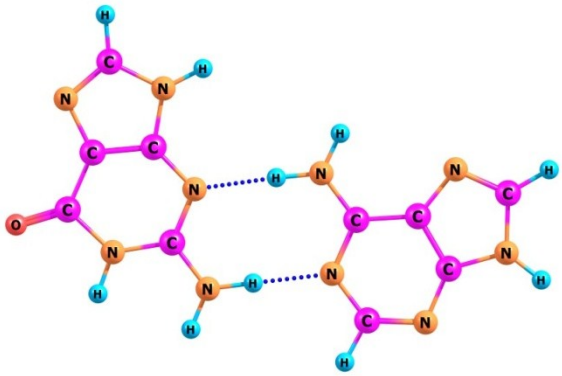

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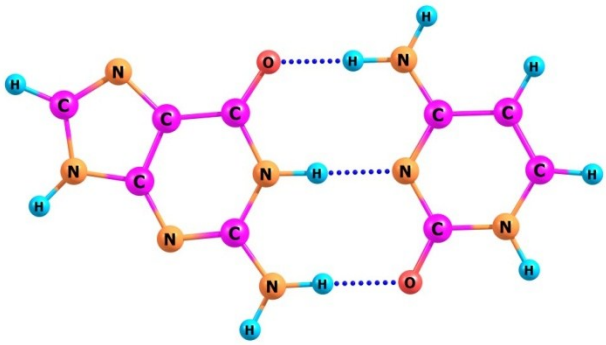

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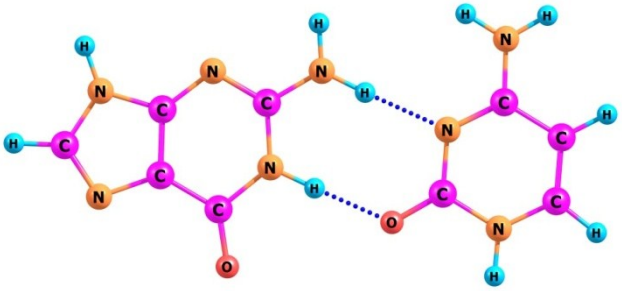

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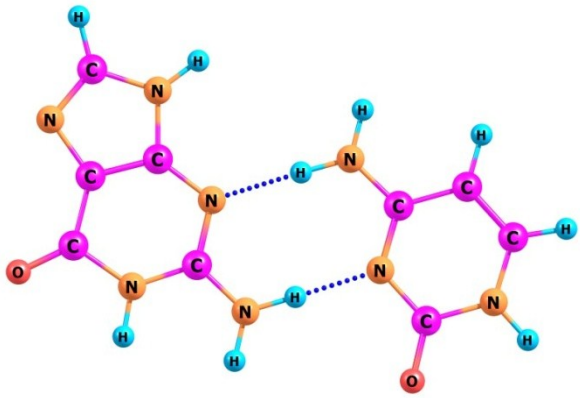

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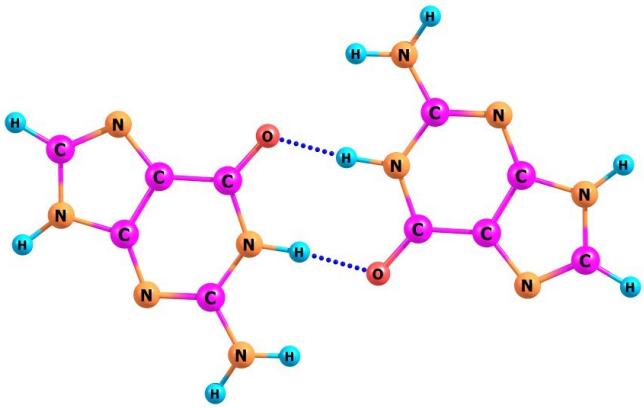

GG1

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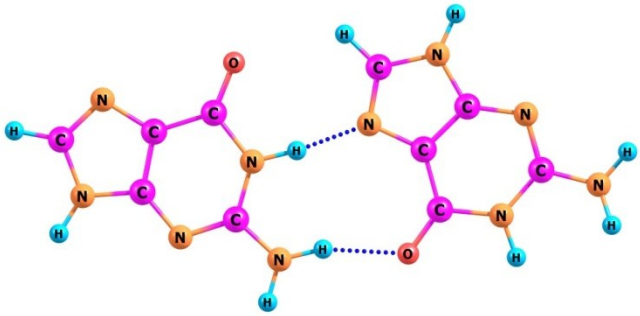

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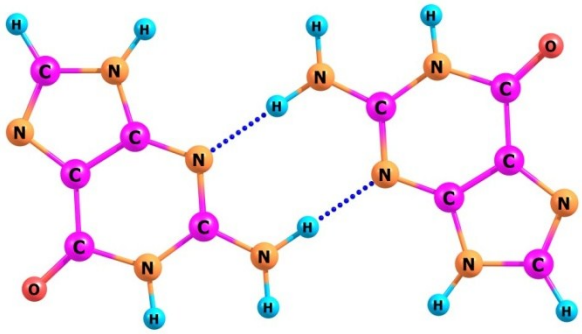

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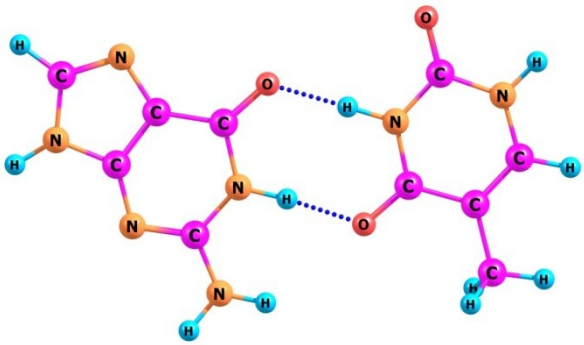

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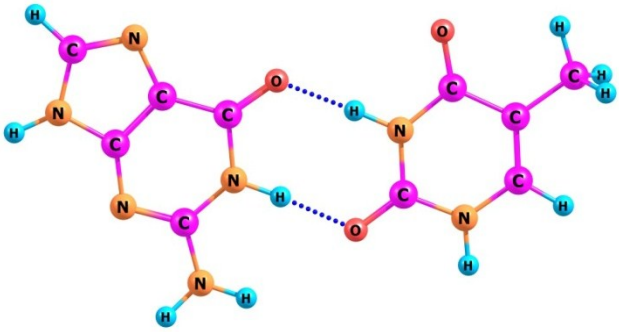

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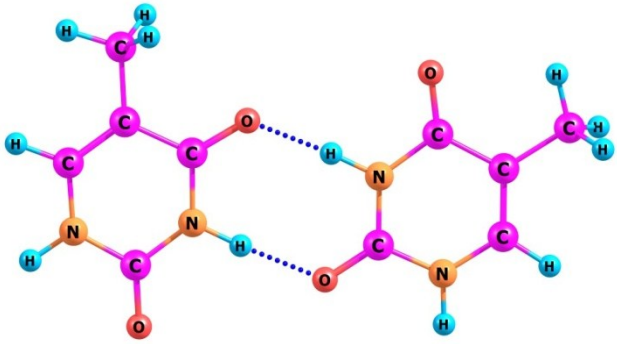

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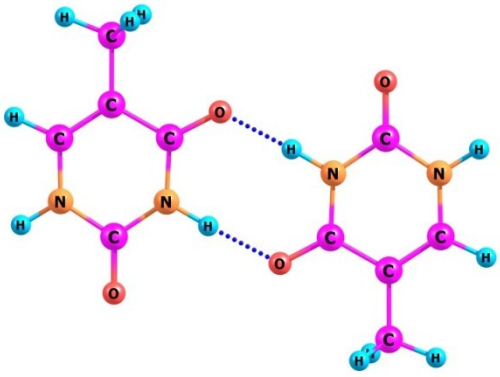

TT2

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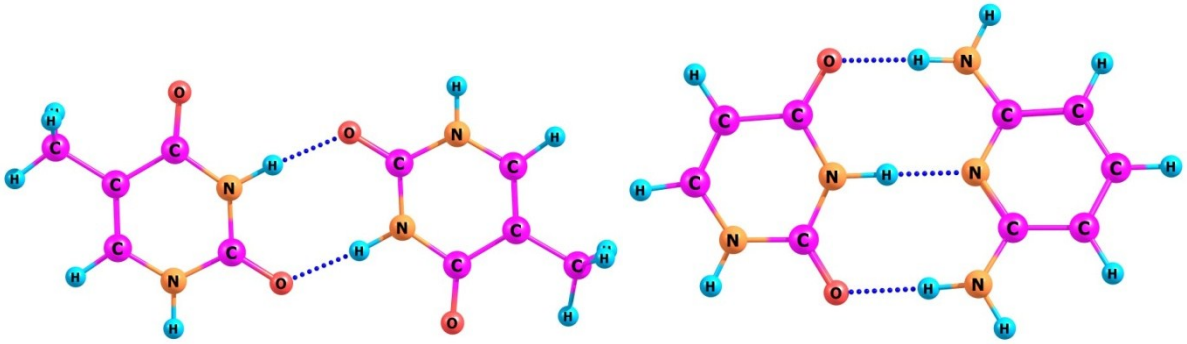


TT3 **U-DAP**

Figure S8. The optimized geometries of 28 base pairs considered by Popelier *et al.* in their QTAIM studies. The same convention of nomenclature of base pairs is followed. Dotted blue lines represent hydrogen bonds.

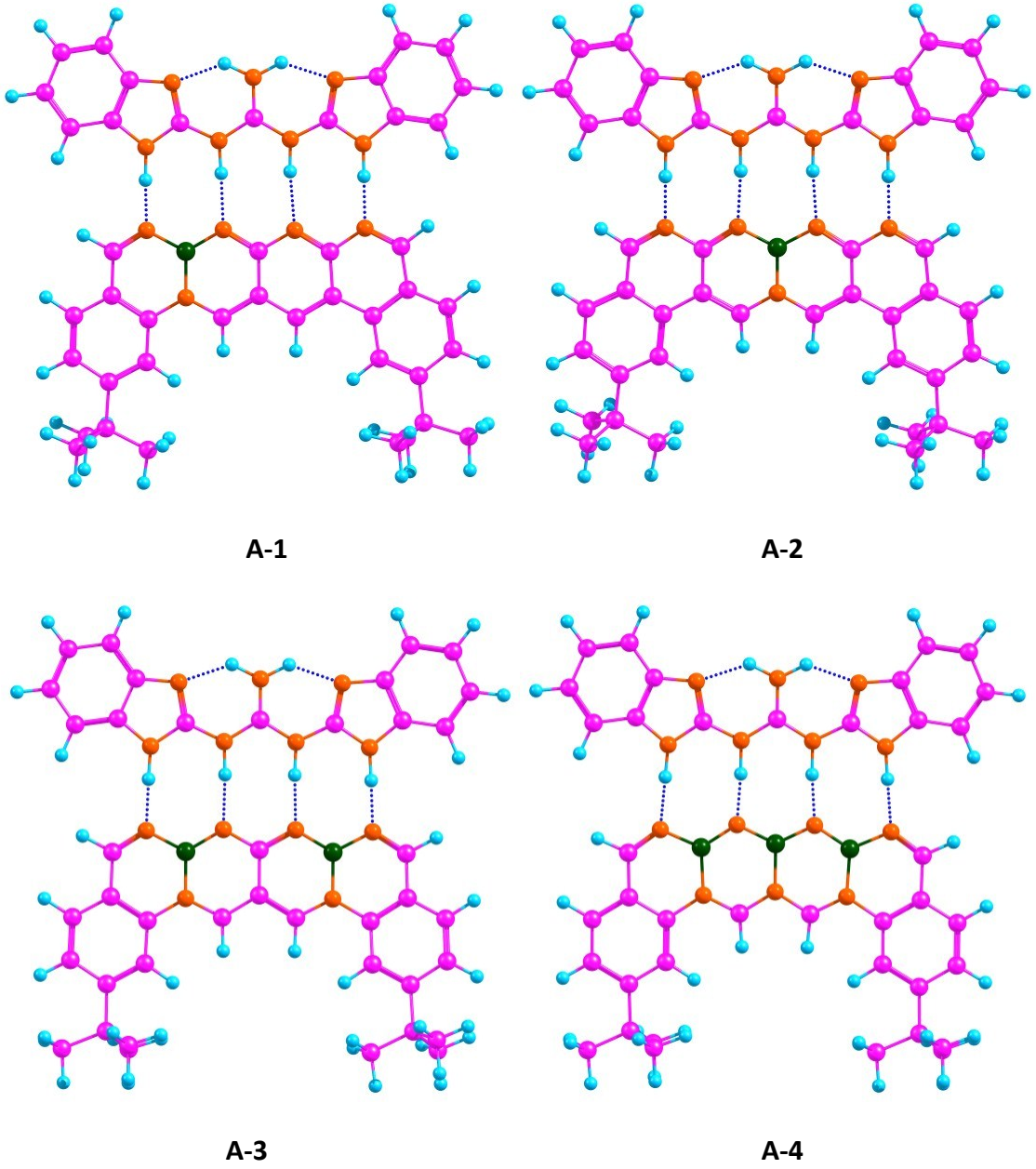
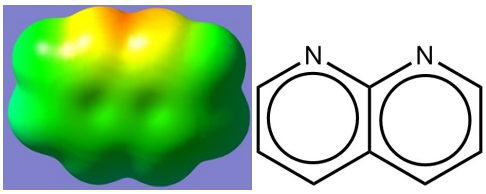
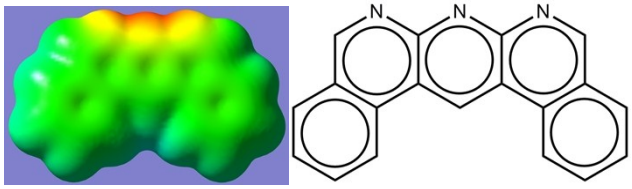


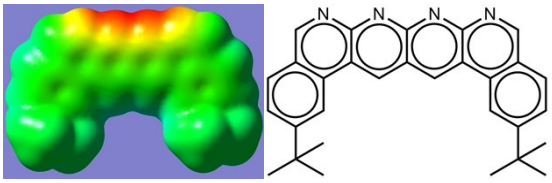
Figure S9. The optimized geometries of newly designed cationic AAAA-DDDD hydrogen bonded complexes, where C-C bond on the middle region of acceptor partner is replaced with the isoelectronic B-N bonds. Pink, cyan, brown and green colors represent carbon, hydrogen, nitrogen and boron atoms respectively, whereas, dotted blue lines represent hydrogen bonds.



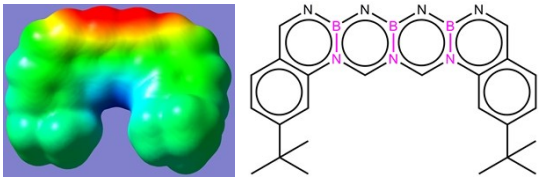
(a)



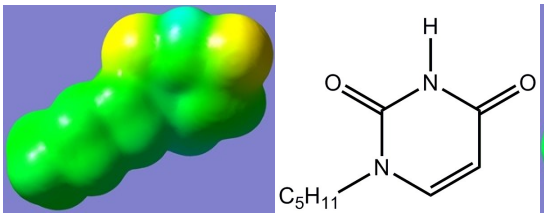
(b)



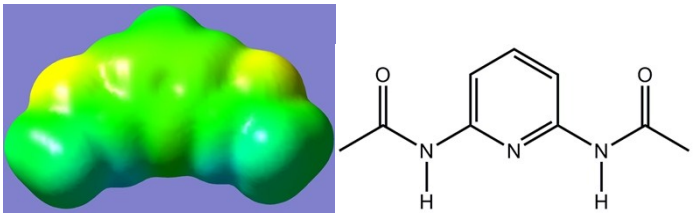
(c)



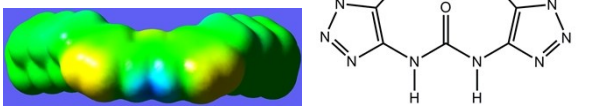
(d)



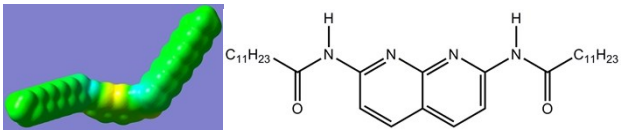
(e)



(f)

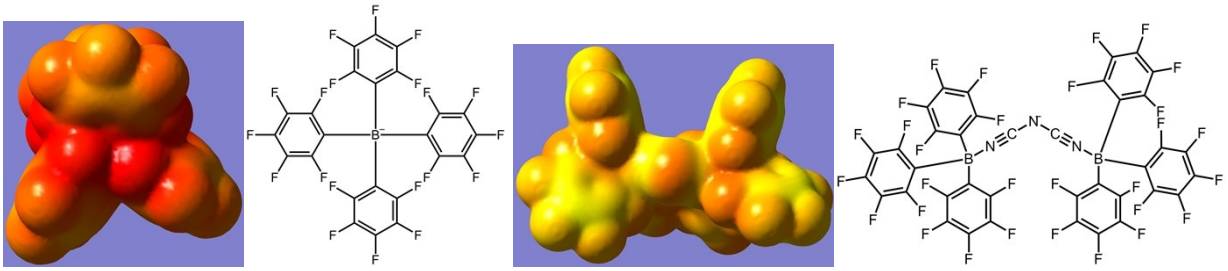


(g)

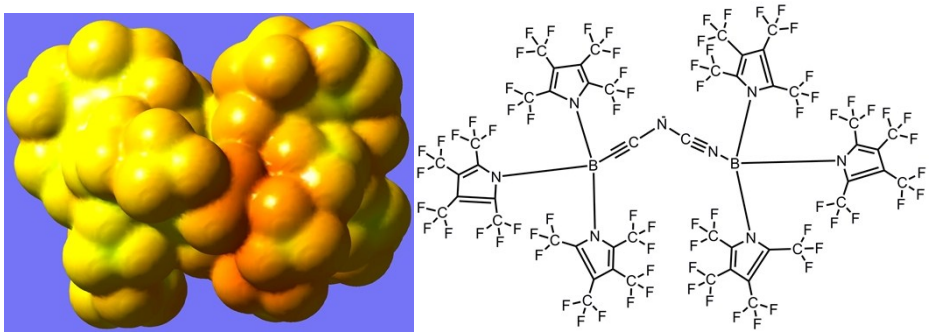


(h)

(Figure continued)



(i) (j)



(k)

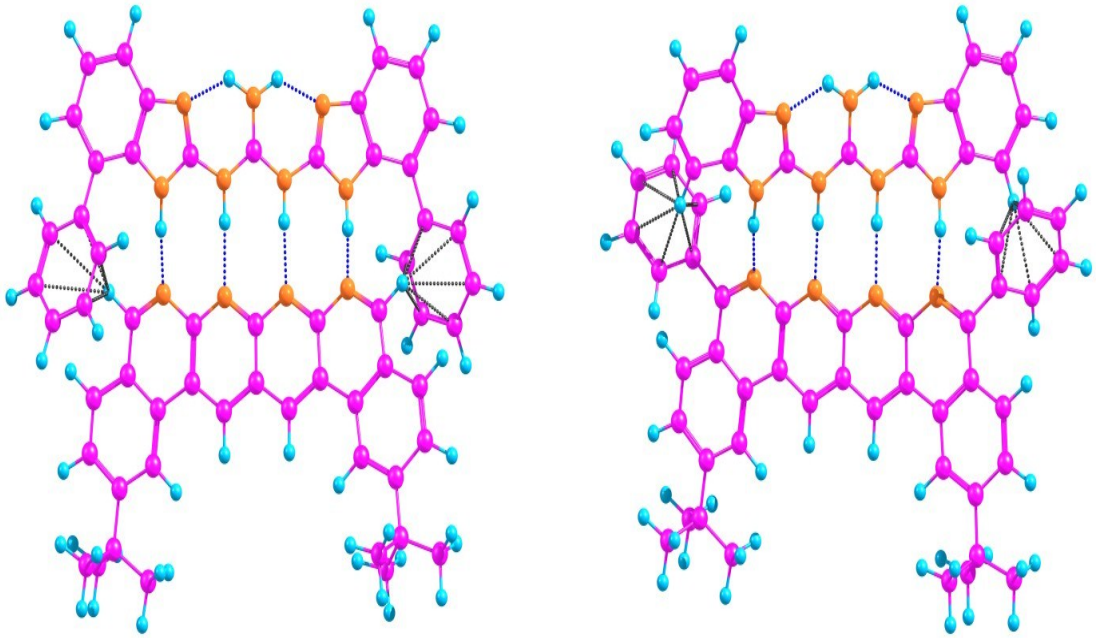
Figure S10. The Molecular Surface electrostatic potential in Hartrees, computed on the 0.0004 au contour of the electron density, using the GaussView software at the CPCM($CHCl_3$)/M062X/6-31G**of theory. The blue color indicates positive electrostatic potential and the red color indicates negative electrostatic potential, whereas, the intermediate colors indicate intermediate electrostatic potential. The color scale was kept uniform in all the cases.

The Molecular surface electrostatic potential map was constructed for a set of representative noncovalent bonding partners containing nitrogen and fluorine on their interactive sites (Figure S10 above), in order to examine whether they possess σ-holes on their potential surface. The obtained electrostatic potential surfaces reveal that none of the moieties considered in this study possess σ-holes on their surface, suggesting that additional treatment of putting extra point charges on the σ-holes positions is not required for an accurate treatment of electrostatic properties in these molecules, as have been proposed in recent studies (see references 63 and 64 in the main manuscript).

A perusal of Figure S10 (above) suggests that the red region of negative potential becomes intensified from (a) to (c), which indicates that the electrostatic attraction for a specific hydrogen bond donor would become increasingly stronger from (a) to (c), which is what has been reported experimentally by Leigh *et al.* (references 23, 25, 26 in the main manuscript). A

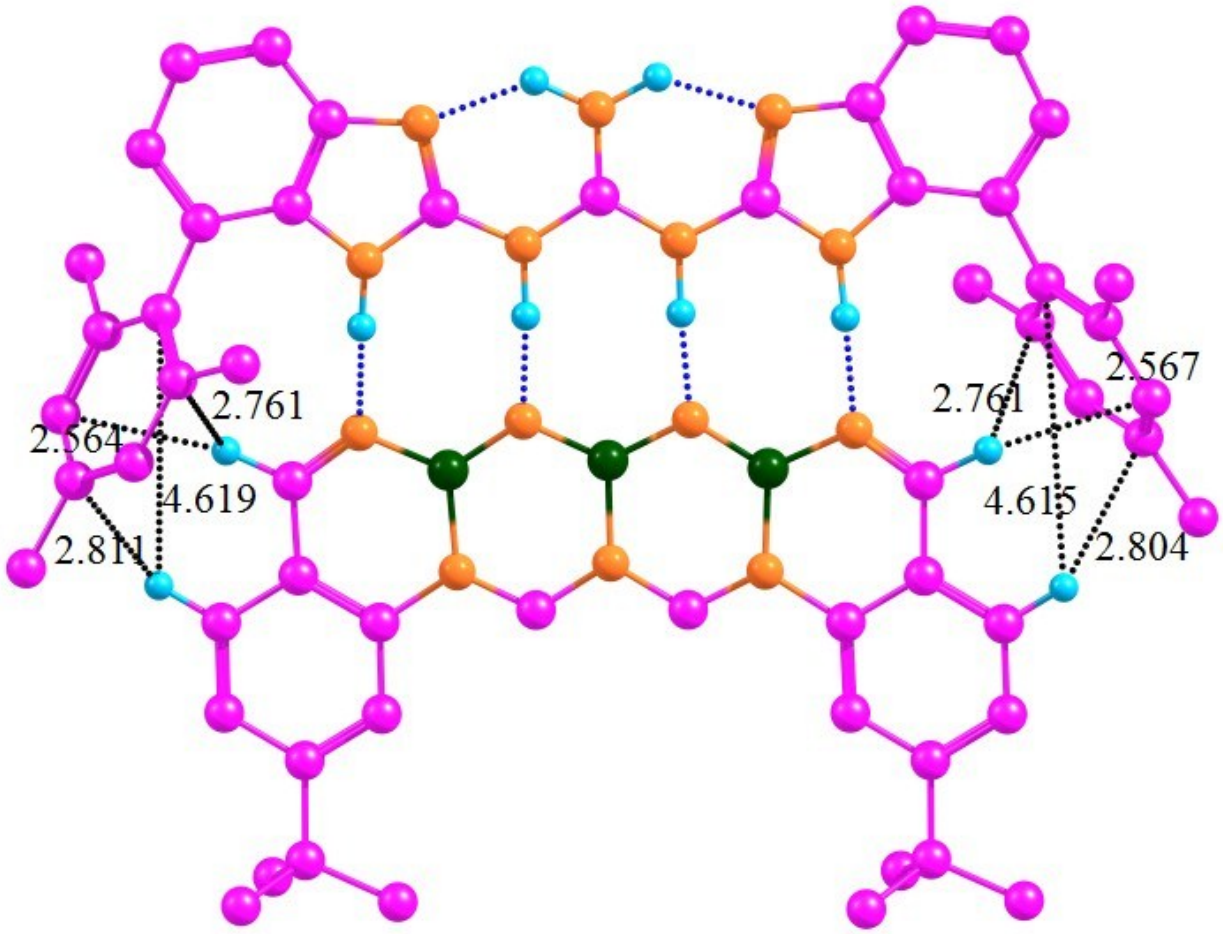
comparison of electrostatic potential surfaces of (c) and (d) further indicates an increase in the negative potential on the binding sites of (d), the newly designed acceptor moiety. This suggests that the binding strength would get stronger for the same donor in (d) in comparison to (c), as obtained in our analysis.

A closer inspection of (i), (j) and (k) in Figure S10 shows increased deterioration of negative potential on the surfaces of these anions on going from (i) to (k), which indicates increasing weaker electrostatic attraction with the cationic zirconocene species. This is reflected in the binding energies of anions with the zirconocene cation. This is what has been observed experimentally by Bochmann et al. (reference 36 in the main manuscript) for (j), and has been obtained by us based on our analysis for (k).



B-1 **B-2**

Figure S11. The optimized geometries of newly designed cationic AAAA-DDDD hydrogen bonded complexes, where hydrogen atoms in frontier lines are replaced with the phenyl groups. Pink, cyan, brown and green colors represent carbon, hydrogen, nitrogen and boron atoms respectively, whereas, dotted blue and black lines represent hydrogen and CH-π bonds respectively.



C

Figure S12. The optimized geometry of hypothetical best case designed cationic AAAA-DDDD hydrogen bonded complex, where hydrogen atoms in frontier lines are replaced with the 2,4,6-trimethylphenyl groups and three C-C bonds in the middle region of acceptor partner is replaced with the isoelectronic B-N bonds. Pink, cyan, brown and green colors represent carbon, hydrogen, nitrogen and boron atoms respectively, whereas, dotted blue and black lines represent hydrogen bond and CH-π interactions respectively. Hydrogen atoms other than those involved in hydrogen bonding and CH-π interactions have been deleted for clarity. The distances shown are the maximum and minimum CH-π distances for each hydrogens.

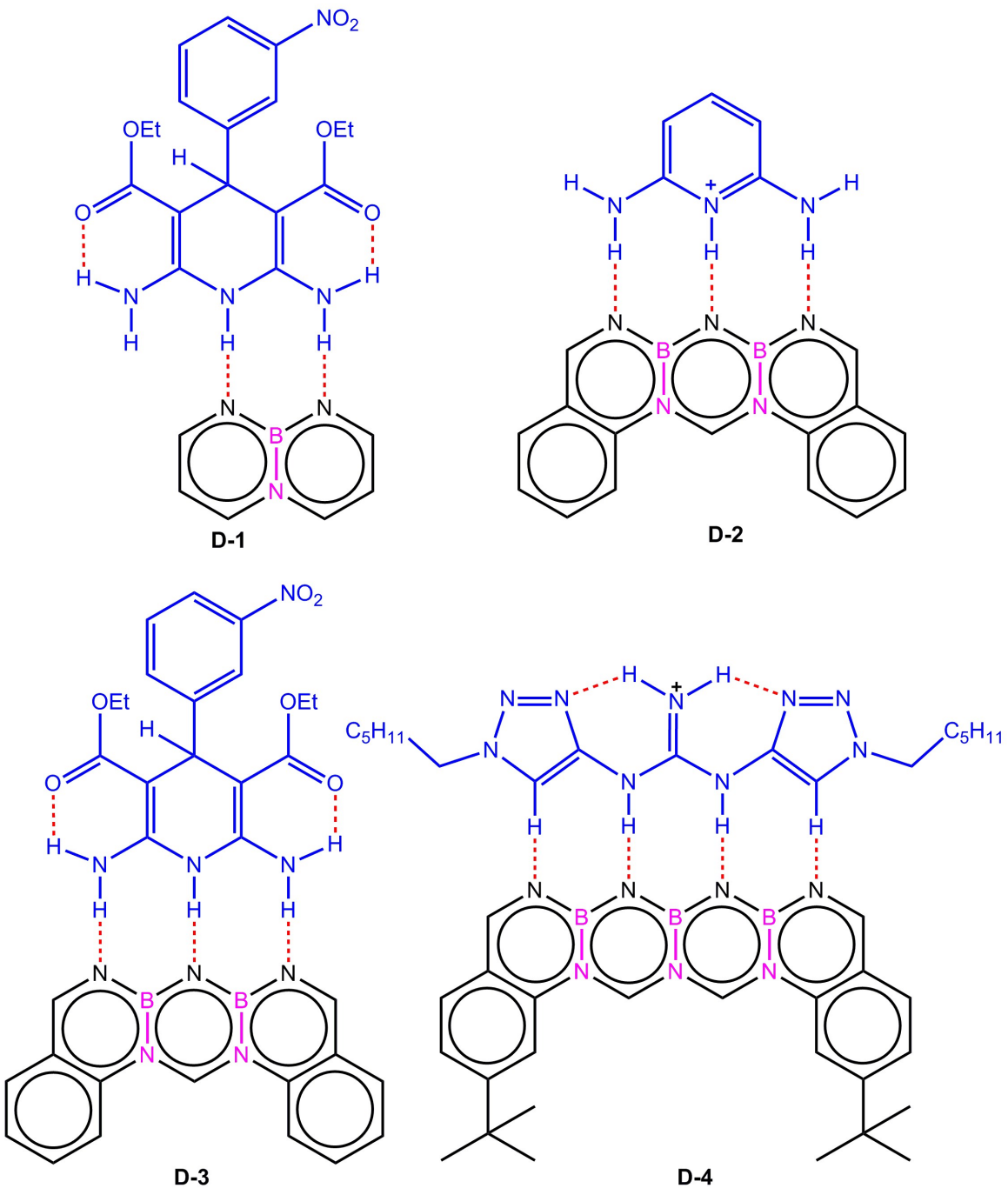


Figure S13. A schematic picture of some newly designed acceptor-donor planer hydrogen bonded complexes based on our electrostatic force analysis, where central C-C bonds on acceptor moieties are replaced by B-N bonds. These complexes have shown improved binding over their parental complexes from where they are derived. Coordinates of optimized geometries are provided in the corresponding section below.

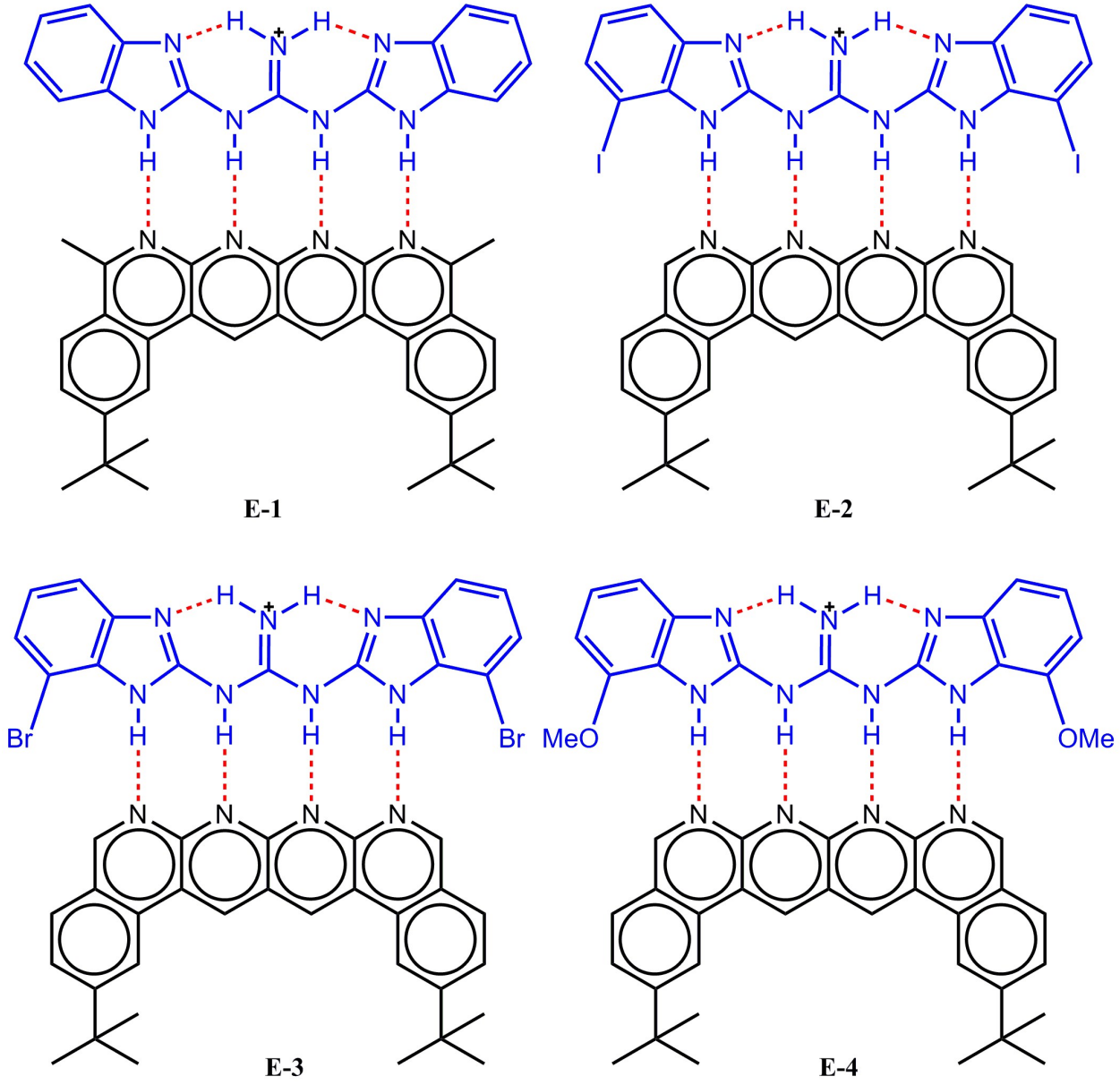


Figure S14. A schematic picture of some newly designed acceptor-donor planer hydrogen bonded complexes, where attractive non-directional dispersive force was exploited for improved binding. These complexes have shown improved binding over their parental complexes from where they are derived. Coordinates of optimized geometries are provided in the corresponding section below.

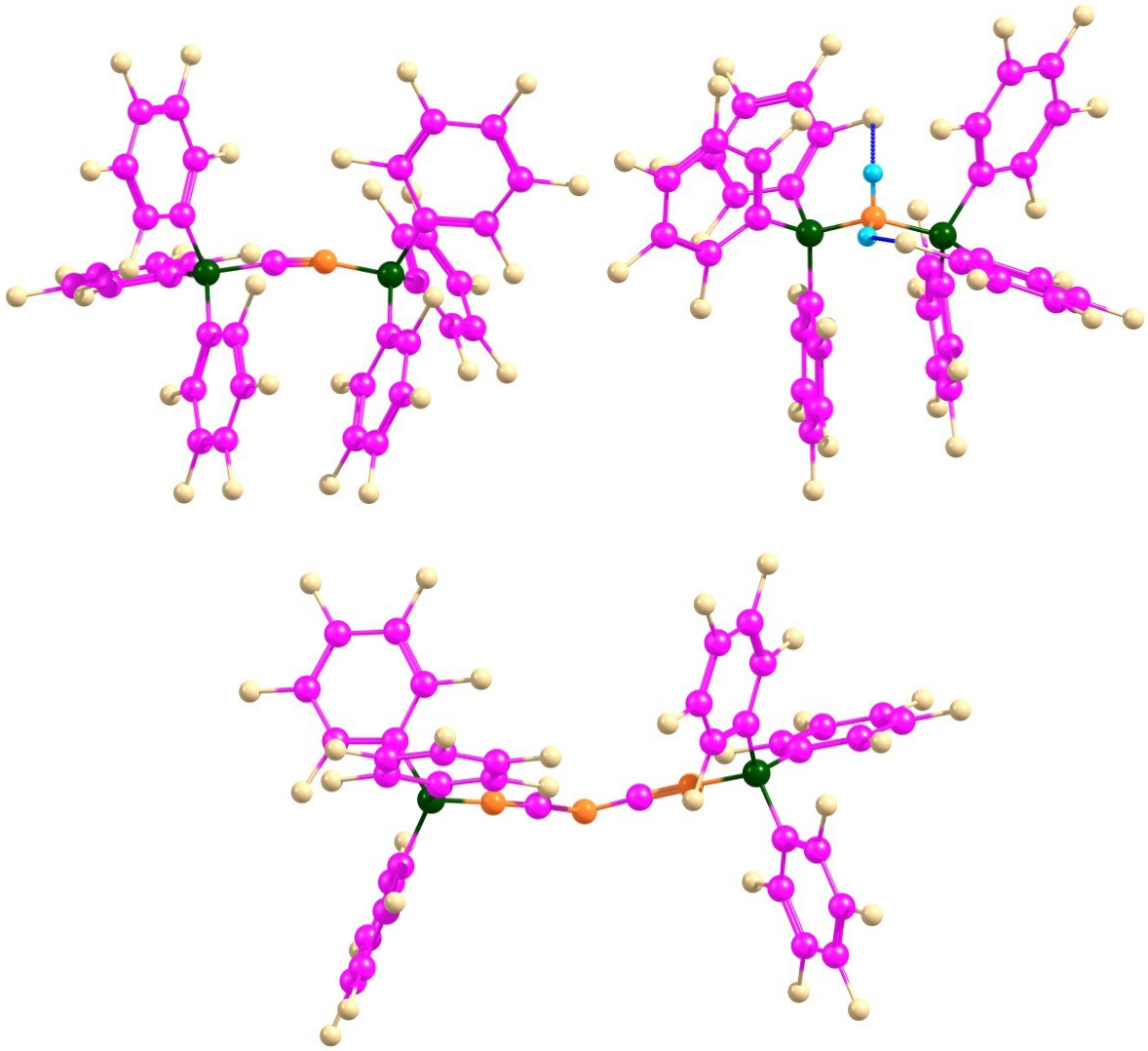


Figure S15. The optimized geometries of Bochmann's anions at the COSMO($CHCl_3$)/PBE/TZVP level of theory using Turbomole 6.4. Pink, cyan, brown, green and white colors represent carbon, hydrogen, nitrogen, boron and fluorine atoms respectively, whereas, dotted blue lines represent hydrogen bonds.

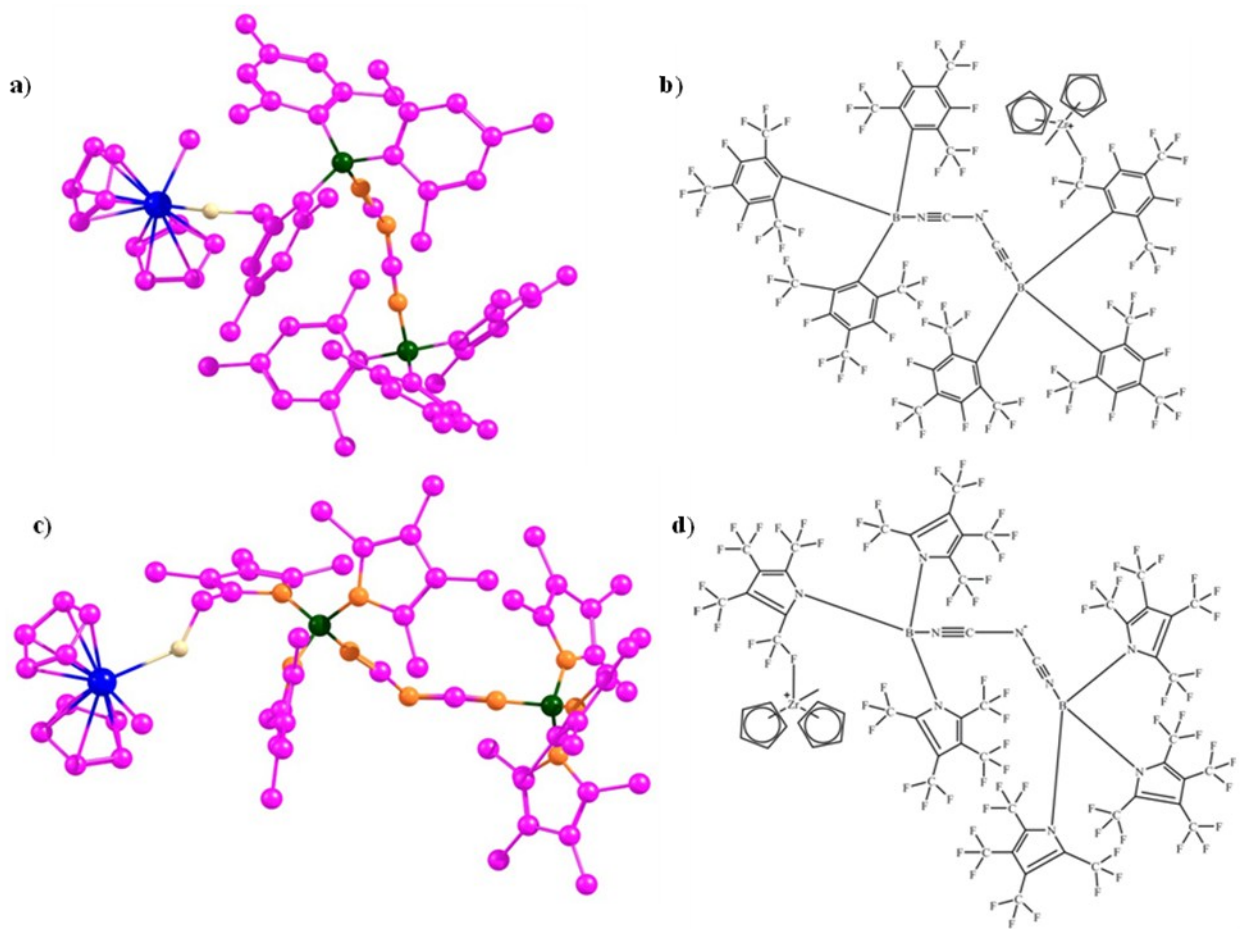


Figure S16. The optimized geometry of the zirconocene complex with newly designed anions. a) anion where *ortho* and *para* fluoro subtstituents are substituted with trifluoro methyl group; b) a schematic picture of a; c) zirconocene complex of best designed anion; d) a schematic picture of c. Pink, white, brown and green colors represent carbon, fluorine, nitrogen and boron atoms respectively. All the hydrogens of the zirconocene and the fluorides of the anions other than the one involved in coordination with the cation have been deleted for clarity.

XYZ coordinates of all the stationary points obtained after full optimization in solvent chloroform.

Turbomole 6.4 geometries

AA-DD (X-1)

C	-3.044305	1.949485	14.204892
C	-1.857839	2.355735	14.815898
C	-0.635427	2.038292	14.204340
C	-0.592268	1.326720	13.000630
C	-1.775243	0.915635	12.383558
C	-2.986178	1.236195	13.004688
C	-1.886314	3.118603	16.138312
C	-1.213443	4.473520	15.990874
C	0.073590	4.657191	16.473404
N	0.696032	3.673552	17.208644
C	0.037003	2.547351	17.668801
C	-1.261689	2.278313	17.241434
N	0.841297	5.767187	16.240311
C	-1.880116	5.532924	15.274963
O	-3.134177	5.165730	14.869785
C	-3.870330	6.135280	14.081147
C	-5.163370	5.470228	13.653364
C	-1.963467	1.134119	17.755411
O	-3.222109	1.018764	17.220542
C	-3.983312	-0.152865	17.605517
C	-5.297203	-0.098469	16.850435
N	0.755740	1.774211	18.512667
N	-4.248798	0.805524	12.373672
O	-4.190336	0.215439	11.283921
O	-1.421871	6.664352	15.016973
O	-1.536372	0.302613	18.582620
O	-5.311845	1.052196	12.963481
N	3.330998	2.819993	19.602276
C	4.114768	3.586253	18.792399
C	5.514210	3.776358	19.038666
C	6.080892	3.145947	20.175087
C	5.271793	2.379656	20.987209
C	3.901147	2.245166	20.653984
N	3.488049	4.160434	17.725693
C	4.210572	4.901899	16.894615
C	5.596544	5.142858	17.053311
C	6.248511	4.580464	18.131088
H	6.122665	5.764408	16.328361
H	5.664346	1.875145	21.870527
H	3.247873	1.632711	21.282468
H	3.671935	5.337842	16.046988
H	1.705762	3.807446	17.449528
H	-2.944719	3.283330	16.382998
H	1.611720	2.148170	18.952840
H	0.245446	0.981208	18.910488
H	-3.403116	-1.054496	17.353050
H	-4.136287	-0.142961	18.696104
H	-5.905429	-0.978938	17.107568
H	-5.865307	0.805314	17.117302
H	-5.126855	-0.096466	15.763607
H	0.314505	6.538311	15.814029
H	1.521595	6.012447	16.955903
H	-4.052097	7.032868	14.693155
H	-3.256343	6.432760	13.216696
H	-5.753865	6.172876	13.046218
H	-4.960501	4.572916	13.050104
H	-5.763224	5.177079	14.527728
H	0.294395	2.355770	14.682899
H	0.367299	1.088373	12.538606
H	-1.770853	0.359253	11.447346
H	-4.004971	2.182993	14.660662
H	7.145024	3.273930	20.386652
H	7.316656	4.739384	18.296912

AAA-DDD, cation, Leigh (X-2)

C	29.643894	11.311791	6.628046
C	30.977919	11.382164	7.081568
C	31.237497	11.156749	8.464138
C	30.179892	10.871996	9.356506
C	28.877654	10.808379	8.886579
C	28.615249	11.029183	7.518391
C	32.591569	11.226685	8.923364
N	33.629354	11.480570	8.164057
C	33.426952	11.702660	6.816850
C	32.116170	11.670752	6.229730
C	32.019512	11.924195	4.859226
C	33.161926	12.192317	4.100914
C	34.425329	12.186948	4.785252
N	34.541343	11.948726	6.104307
N	35.614177	12.429227	4.126592
C	35.581232	12.682542	2.840848
C	34.392526	12.726181	2.044077
C	33.142022	12.470761	2.677119
C	31.972064	12.500488	1.889332
C	32.049965	12.772626	0.528701
C	33.290810	13.025343	-0.092676
C	34.454236	13.003633	0.660136
N	38.169579	11.941342	5.276707
C	38.368453	11.838814	6.601957
N	37.252305	11.807717	7.407372
C	37.316803	11.689711	8.777589
C	38.578433	11.592203	9.387541
C	39.717093	11.622945	8.585674
C	39.635611	11.745214	7.200665
N	36.153866	11.695158	9.452045
H	32.789043	11.057310	9.988342
H	30.404948	10.704008	10.412250
H	28.055546	10.587997	9.569226
H	27.588380	10.976647	7.152387
H	29.406957	11.477241	5.576751
H	31.042533	11.912672	4.376138
H	30.996863	12.310360	2.338525
H	31.136147	12.790192	-0.067867
H	33.330674	13.234989	-1.162560
H	35.425648	13.195895	0.199177
H	36.543504	12.867701	2.349583
H	36.308235	11.873098	6.955391
H	35.231980	11.629291	8.960508
H	36.190290	11.539288	10.453581
H	38.637762	11.495630	10.470511
H	40.699733	11.549701	9.055687
H	40.522881	11.772074	6.570187
H	37.223284	12.132489	4.874278
H	38.986432	12.026306	4.681746

AAA-DDD, neutral, Leigh (X-3)

C	6.272532	4.942383	18.665328
C	5.623274	3.806798	19.156864
C	4.246636	3.620761	18.787377
N	3.575941	4.483753	18.005718
C	4.217618	5.572464	17.549275
C	5.594845	5.853516	17.851068
C	6.252892	2.816537	20.009648
C	5.456174	1.711835	20.425416
C	4.093975	1.646079	19.982421
N	3.512568	2.532715	19.215301
C	6.195865	7.053050	17.298282
C	5.999779	0.708207	21.257100
H	3.482809	0.794707	20.304794
N	3.453160	6.410918	16.762768
C	7.592755	2.881442	20.447682
H	7.317817	5.118956	18.919342
C	4.007657	7.490436	16.272782
H	3.373295	8.133340	15.651216
C	5.369644	7.883532	16.488420
C	5.884809	9.066085	15.912847
C	7.205326	9.425333	16.133536
H	5.228936	9.685181	15.296300
H	7.610173	10.336905	15.690811
C	8.028339	8.606866	16.935105
C	7.536282	7.441025	17.509423
H	9.067663	8.892698	17.106917
H	8.197231	6.829514	18.124734
C	7.318898	0.793780	21.674149
H	5.366153	-0.127758	21.562082
H	7.745114	0.021937	22.316992
C	8.112591	1.885566	21.265218
H	8.231623	3.713491	20.149686
H	9.150873	1.950218	21.595986
N	0.725496	2.087924	18.546716
C	0.020579	2.764289	17.619631
N	0.677023	3.837253	17.034185
C	0.026622	4.760917	16.228804
C	-1.282998	4.524833	15.806304
C	-1.949196	3.192369	16.095972
C	-1.286913	2.451053	17.242301
C	-1.956946	2.323375	14.839370
C	-3.158733	1.962461	14.230069
C	-3.132647	1.164860	13.082800
C	-1.937906	0.708642	12.517052
C	-0.739265	1.075231	13.131722
C	-0.751148	1.874400	14.280216
N	-4.410306	0.793835	12.447043
O	-5.461138	1.223005	12.948546
C	-1.953696	5.488207	14.979608
O	-1.499783	6.579089	14.571400
N	0.743539	5.852675	15.902710
C	-1.952734	1.324815	17.833896
O	-1.497825	0.549105	18.701980
O	-3.222035	5.083209	14.642293
C	-3.954684	5.939438	13.733535
C	-5.265496	5.242446	13.425360
O	-3.216061	1.149224	17.324346
C	-3.937537	-0.022237	17.774807
C	-5.254822	-0.050193	17.023963
O	-4.379256	0.071057	11.438422
H	1.631061	4.063422	17.363565
H	-3.001268	3.375479	16.356152
H	1.712104	2.314585	18.766362
H	0.249040	1.270759	18.939291
H	-3.331322	-0.918450	17.568318
H	-4.088446	0.039959	18.864167
H	-5.832818	-0.936271	17.327739
H	-5.851485	0.847183	17.244930
H	-5.085882	-0.098509	15.937933
H	0.251988	6.532218	15.314582
H	-4.114075	6.920970	14.208232
H	-3.352539	6.097994	12.824944
H	-5.855091	5.858883	12.729903
H	-5.089259	4.261109	12.959760
H	-5.854967	5.092145	14.342228
H	0.190479	2.155313	14.758270
H	0.208092	0.733457	12.711088
H	-1.958259	0.087572	11.622666
H	-4.106860	2.299111	14.645981
H	1.693636	6.023271	16.278912

AAA-DDD, OH, Leigh (**X-4**)

N	1.076790	0.696409	18.874651
C	1.741923	-0.049032	19.829593
C	1.100787	-1.094483	20.575574
C	-0.291394	-1.388634	20.296532

C	-0.937504	-0.600485	19.301001
C	-0.184179	0.428025	18.643476
N	3.030431	0.276807	20.009684
C	3.766912	-0.384913	20.919286
C	3.211735	-1.428285	21.736931
C	1.869368	-1.761533	21.534645
C	4.070948	-2.070129	22.713463
C	5.422807	-1.627134	22.780525
C	5.848907	-0.584863	21.889269
N	5.086967	0.011554	21.007686
C	3.653337	-3.096046	23.587335
C	4.548511	-3.654406	24.491251
C	5.886058	-3.212014	24.554328
C	6.319415	-2.205404	23.705130
C	-2.292760	-0.829658	18.975301
C	-3.001549	-1.830080	19.622349
C	-2.365299	-2.615210	20.606604
C	-1.033825	-2.401009	20.940739
H	6.893660	-0.254166	21.933279
H	1.416270	-2.554647	22.129679
H	-0.687230	1.041446	17.887354
H	-2.766226	-0.211088	18.209481
H	-4.048058	-2.013011	19.373404
H	-2.925530	-3.403428	21.113060
H	-0.568182	-3.025050	21.704243
H	7.351363	-1.848514	23.737160
H	6.574764	-3.662499	25.270977
H	2.624509	-3.457742	23.563443
H	4.211036	-4.446840	25.162055
C	5.077167	2.913666	18.583593
C	6.455819	3.208642	18.533564
C	6.881545	4.532809	18.673280
C	5.970790	5.581598	18.873179
C	4.611308	5.252071	18.962239
C	4.140641	3.937068	18.832414
C	7.427027	2.059052	18.423513
O	7.408919	1.211817	19.591921
C	6.436705	7.012774	18.974184
C	2.666038	3.641178	18.980873
O	2.079168	3.085289	17.794348
O	4.732707	1.608839	18.376248
H	3.879463	6.045759	19.145598
H	7.955069	4.745459	18.641330
H	1.777647	2.172729	18.047843
H	3.964471	1.300634	18.948880
H	6.475766	0.926310	19.730795
H	7.386619	7.085737	19.526174
H	6.605476	7.448660	17.974458
H	5.688835	7.637747	19.484896
H	2.147164	4.582371	19.236495
H	2.512807	2.942349	19.824951
H	8.453907	2.443763	18.338951
H	7.203149	1.458762	17.522479

AAA-DDD, Cation, model (**X-5**)

C	6.192566	4.945133	18.646510
C	5.550390	3.813042	19.133199
C	4.201007	3.564079	18.805824
C	3.523080	4.496860	17.968811
C	4.190076	5.643533	17.483201
C	5.515784	5.866216	17.820083
C	2.154679	4.243213	17.633035
N	1.464367	3.207576	18.042439
C	2.076627	2.280197	18.859318
C	3.447515	2.413666	19.267596
N	1.295067	1.253172	19.238073
C	1.821706	0.305028	20.033542
C	3.180651	0.337719	20.497923
C	3.971613	1.416128	20.093780
C	3.649635	-0.738607	21.350662
C	2.719284	-1.767673	21.676722
C	1.391422	-1.679056	21.149014
N	0.957128	-0.713287	20.377039
C	3.102234	-2.848102	22.502432
C	4.393557	-2.912031	23.001687
C	5.319185	-1.896749	22.681514
C	4.957809	-0.827123	21.871082
H	1.634152	4.959619	16.986955
H	5.007551	1.479832	20.426826
H	0.675590	-2.469658	21.401359
H	2.369136	-3.622976	22.737224
H	4.697014	-3.742888	23.640233
H	6.335384	-1.951225	23.076187
H	5.696942	-0.058910	21.642798
H	3.647019	6.343703	16.844579
H	6.037533	6.749771	17.449188
H	6.102155	3.120858	19.769881
H	7.237002	5.123944	18.908540
N	-1.760436	-0.783881	19.644738
C	-2.397771	0.103093	18.889167
N	-1.637997	1.142600	18.416442
C	-2.117159	2.142700	17.609178
C	-3.495600	2.147399	17.232209
C	-4.338227	1.077813	17.721300
C	-3.785349	0.032916	18.555437
N	-1.230207	3.056212	17.230332
C	-4.539248	-1.106956	19.096135
O	-5.860718	-1.136703	18.764777
C	-6.642942	-2.262108	19.281179
C	-8.069633	-2.059198	18.819802
N	-5.636869	1.052733	17.396562
C	-3.944225	3.255042	16.376113
O	-5.271743	3.245254	16.066219
C	-5.756690	4.329250	15.208998
C	-7.249104	4.135183	15.049721
O	-4.062615	-2.003167	19.805159
O	-3.217216	4.157769	15.941730
H	-0.626355	1.169964	18.682203
H	-0.232050	3.041868	17.556338
H	-1.598180	3.802163	16.629265
H	-5.510105	5.285980	15.690620
H	-5.222620	4.272314	14.249870
H	-7.644573	4.931058	14.401450
H	-7.476503	3.166371	14.580861
H	-7.762127	4.195323	16.020764
H	-2.337511	-1.557457	19.993794
H	-6.205212	-3.191462	18.889788
H	-6.556041	-2.267956	20.377005
H	-8.685853	-2.891451	19.191076
H	-8.483759	-1.120570	19.216680
H	-8.134612	-2.046398	17.721717
H	-0.738024	-0.701984	19.870303
H	-6.012415	1.792478	16.805823
H	-6.218265	0.291467	17.742492

AAA-DDD, anion, model (**X-7**)

C	6.230690	4.991475	18.625927
C	5.568026	3.843772	19.114165
C	4.203166	3.644893	18.754861
C	3.538550	4.579610	17.928755
C	4.211255	5.697977	17.462559
C	5.562632	5.900242	17.815499
C	3.528744	2.481117	19.249541
N	4.081388	1.574429	20.018925
C	5.398021	1.725834	20.390281
C	6.191562	2.845943	19.964210
C	7.518431	2.906573	20.394442
C	8.051810	1.902296	21.216092
C	7.162180	0.825832	21.583668
N	5.886375	0.747787	21.181421
N	7.583576	-0.216309	22.393719
C	8.815919	-0.227088	22.831709
C	9.803130	0.780013	22.537334
C	9.398073	1.871498	21.706272
C	11.100636	0.716503	23.027793
C	12.062722	1.746331	22.709575
N	11.636044	2.812615	21.889331
C	10.393936	2.844502	21.438117
H	9.105077	-1.072126	23.468975
H	8.152089	3.740106	20.091105
H	2.479148	2.325845	18.973307
H	2.492079	4.403499	17.667045
H	3.700774	6.421623	16.824774
H	6.090761	6.782066	17.447257
H	7.275021	5.173484	18.882160
H	11.413789	-0.115554	23.662864
O	13.247806	1.727808	23.130050
H	10.141342	3.706138	20.806768
N	5.924945	-2.399750	23.170586
C	4.673764	-2.660874	22.770686
N	4.116842	-1.702762	21.958464
C	2.833594	-1.763159	21.459763
C	2.001953	-2.870468	21.757667
C	2.527925	-3.972736	22.608772
C	3.925179	-3.814015	23.123141
C	0.656133	-2.839609	21.182304
O	-0.142267	-3.899270	21.461018
C	-1.471274	-3.852111	20.883458
C	-2.174506	-5.130162	21.298452
N	2.483102	-0.712796	20.703102
C	4.611114	-4.780090	23.970859
O	3.898405	-5.911194	24.277827
C	4.567747	-6.886783	25.122001
C	3.607086	-8.044214	25.307826
N	1.763162	-4.998514	22.863624
O	5.767620	-4.666750	24.427322
O	0.208383	-1.913719	20.464563
H	4.696181	-0.876066	21.714066
H	6.457239	-1.562500	22.846744
H	6.344853	-3.121263	23.766413
H	5.501360	-7.202627	24.632498
H	4.828940	-6.410867	26.079517
H	4.076797	-8.807343	25.947105
H	2.677146	-7.709554	25.790815
H	3.356793	-8.506069	24.341218
H	1.525027	-0.759064	20.334605
H	-1.998563	-2.957727	21.251992
H	-1.392023	-3.767212	19.788221
H	-3.193963	-5.139201	20.882966
H	-1.635022	-6.012219	20.923206
H	-2.241029	-5.202246	22.393872
H	3.126399	0.082694	20.513208
H	2.277344	-5.652598	23.457725

AAA-DDD, ion pair, model (**X-8**)

N	4.907276	0.542547	20.933093
C	3.622237	0.157096	20.631208
C	3.064329	-1.079300	21.104640
C	3.898262	-1.936346	21.928631
C	5.222493	-1.493058	22.215736
C	5.654301	-0.238507	21.678972
C	1.751387	-1.382951	20.742155
C	1.005133	-0.503568	19.941480
C	1.665843	0.711305	19.527096
N	2.926868	1.021916	19.860940
C	-0.342399	-0.725136	19.514809
C	-0.979806	0.263485	18.698911
C	-0.213244	1.431399	18.359962
N	1.020147	1.650256	18.740807
C	-2.285040	0.080307	18.264207
C	-3.023029	-1.108978	18.624869
N	-2.371307	-2.066947	19.432336
C	-1.129138	-1.863115	19.830272
C	6.084242	-2.282191	23.011564
C	5.645047	-3.494895	23.518312
C	4.335188	-3.938665	23.237429
C	3.475751	-3.175296	22.457458
H	-0.681077	2.204107	17.737516
H	1.295323	-2.313089	21.080315
H	6.672088	0.105215	21.895366
H	7.094758	-1.920844	23.216971
H	6.307164	-4.107198	24.132721
H	3.991367	-4.894383	23.637551
H	2.469032	-3.543797	22.257486
H	-2.774806	0.832630	17.641446

O	-4.203359	-1.317261	18.252009
H	-0.695995	-2.655774	20.454548
C	6.186965	4.935318	18.651406
C	5.524979	3.768211	19.150767
N	4.213714	3.539047	18.822888
C	3.457362	4.375237	18.041014
C	4.046464	5.562916	17.499969
C	5.431983	5.836871	17.808870
N	6.094681	2.858807	19.931679
N	2.199958	4.002893	17.843607
C	3.184134	6.408147	16.664039
O	1.990913	6.189315	16.418981
N	6.019683	6.935292	17.314341
C	7.590588	5.118674	19.039858
O	8.237221	4.353112	19.767354
O	8.191967	6.236190	18.534592
C	9.590441	6.452211	18.904336
C	10.042844	7.717713	18.207904
O	3.790808	7.510967	16.132717
C	2.958639	8.378187	15.299087
C	3.848011	9.494492	14.795435
H	3.757614	2.668347	19.197336
H	1.805407	3.099051	18.229834
H	1.643041	4.633537	17.257266
H	2.543395	7.775123	14.479256
H	2.127065	8.751964	15.913847
H	3.251183	10.170987	14.165965
H	4.263548	10.078077	15.630328
H	4.674264	9.097314	14.187182
H	7.075265	3.040169	20.170969
H	9.648435	6.535471	19.999202
H	10.171176	5.573438	18.589702
H	11.094101	7.912207	18.467188
H	9.970930	7.614798	17.115053
H	9.443293	8.582475	18.528501
H	5.580192	2.005287	20.284763
H	5.476828	7.559070	16.720169
H	6.995056	7.118132	17.541686

AAA-DDD, neutral, model (**X-6**)

N	4.883885	0.520032	20.939715
C	3.595276	0.125227	20.641281
C	3.046268	-1.113988	21.120104
C	3.878737	-1.970222	21.943677
C	5.200938	-1.521382	22.224133
C	5.624898	-0.262746	21.682293
C	1.731804	-1.417722	20.756902
C	0.993311	-0.540314	19.959015
C	1.639798	0.672145	19.537671
N	2.903013	0.984575	19.874035
C	-0.372803	-0.782461	19.535557
C	-0.989803	0.210123	18.721394
C	-0.232145	1.376922	18.374493
N	1.000122	1.607477	18.749850
C	-2.316885	0.042925	18.268466
C	-3.028853	-1.094344	18.615696
C	-2.423177	-2.080246	19.422165
C	-1.118866	-1.930630	19.876540
C	6.069797	-2.302305	23.017910
C	5.636926	-3.515152	23.531074
C	4.328065	-3.964201	23.257199
C	3.461482	-3.208219	22.477498
H	-0.708971	2.140267	17.748190
H	1.278982	-2.348698	21.097789
H	6.643359	0.080456	21.898796
H	7.079368	-1.935975	23.217361
H	6.303288	-4.122951	24.145190
H	3.990086	-4.919416	23.663210
H	2.455723	-3.582354	22.283454
H	-2.766320	0.819424	17.645248
H	-4.054312	-1.230110	18.268277
H	-0.679454	-2.710837	20.499357
H	-2.987070	-2.974696	19.693704
C	6.236943	5.005787	18.618089
C	5.577217	3.855970	19.109246
N	4.257024	3.620812	18.788456
C	3.491381	4.456362	18.012067
C	4.060670	5.632242	17.463763
C	5.496205	5.958272	17.745656
N	6.129549	2.920653	19.897677
N	2.220416	4.061071	17.845045
C	3.172369	6.440774	16.636891
O	1.969960	6.198665	16.400842
N	6.115462	7.007742	17.282873
C	7.637425	5.165666	19.019137
O	8.260329	4.364774	19.755940
O	8.276358	6.261032	18.547337
C	9.662800	6.403529	18.953373
C	10.181864	7.670250	18.301708
O	3.735204	7.556918	16.079619
C	2.863676	8.377917	15.253827
C	3.701633	9.530533	14.738596
H	3.811828	2.766821	19.166289
H	1.861024	3.163588	18.222032
H	1.654718	4.677481	17.250739
H	2.463897	7.761189	14.434843
H	2.016947	8.724377	15.865733
H	3.076635	10.180832	14.108195
H	4.099320	10.130271	15.570564
H	4.543271	9.163494	14.132729
H	7.113222	3.098448	20.138177
H	9.716350	6.456924	20.052303
H	10.229917	5.516040	18.631425
H	11.234703	7.822436	18.585097
H	10.120509	7.599030	17.205938
H	9.600654	8.544829	18.628575
H	5.603056	2.094024	20.234625
H	5.465197	7.549662	16.709390

AAA-DDD, EWG, model (**X-9**)

C	3.391302	-3.116342	22.765727
C	3.863863	-2.008985	22.034295
C	5.233151	-1.623365	22.240630
C	6.086868	-2.424933	23.025257
C	5.604533	-3.566382	23.652911
C	4.250855	-3.900365	23.531881
C	5.610190	-0.340000	21.712606
N	4.841348	0.491832	21.101217
C	3.554354	0.119212	20.796519
C	3.046660	-1.167717	21.179404
C	1.824391	-1.525149	20.584421
C	1.005278	-0.581515	19.941889
C	1.642871	0.668025	19.641614
N	2.878653	0.994604	20.040880
N	1.044362	1.584360	18.812516
C	-0.082482	1.297560	18.262074
C	-0.879904	0.127929	18.508552
C	-0.347817	-0.801932	19.466119
C	-2.164520	-0.067664	17.964410
C	-2.955022	-1.129549	18.383924
C	-2.485069	-1.982435	19.389612
C	-1.220696	-1.798033	19.944991
F	-0.567427	2.217512	17.416260
F	1.495265	-2.819275	20.512337
F	6.872896	0.068053	21.903154
F	7.372596	-2.108518	23.221054
F	6.407958	-4.324692	24.403494
F	3.776584	-4.955502	24.198291
F	2.090191	-3.436781	22.814234
F	-2.679528	0.766142	17.053001
F	-4.172690	-1.318371	17.868611
F	-0.908243	-2.574237	20.992770
F	-3.279882	-2.952078	19.847697
N	2.160537	4.257251	18.212432
C	3.488647	4.451611	18.094000
N	4.281121	3.504174	18.707654
C	5.632443	3.691909	18.937026
C	6.292146	4.771137	18.332220
C	5.569933	5.549965	17.299767
C	4.086459	5.528602	17.410616
C	7.660823	5.052758	18.749944
O	8.101044	6.291083	18.422996
C	9.455025	6.617205	18.828729
C	9.763060	7.991276	18.268079
N	6.213020	2.781215	19.741416
C	3.203375	6.498881	16.782605
O	3.849909	7.562764	16.221315
C	3.006880	8.567342	15.593180
C	3.927520	9.632059	15.033396
N	6.251533	6.149353	16.369303
O	1.958935	6.436344	16.744605
O	8.378784	4.276070	19.414006
H	3.816083	2.714032	19.180699
H	1.792719	3.345539	18.510470
H	1.586874	4.901767	17.656860
H	2.404811	8.086841	14.806934
H	2.318045	8.974799	16.348962
H	3.325581	10.416502	14.550470
H	4.524521	10.094061	15.833319
H	4.610619	9.207186	14.282965
H	7.209756	2.938519	19.924791
H	9.518474	6.598990	19.928642
H	10.143126	5.852034	18.437094
H	10.786813	8.280051	18.550177
H	9.686914	7.988204	17.171031
H	9.065966	8.743633	18.665866
H	5.664361	2.093709	20.268331
H	5.607592	6.656896	15.753161

AAA-DDD, wd ester, model (**X-10**)

C	6.106308	5.154754	18.934353
C	5.475232	3.961742	19.346462
C	4.091318	3.790144	19.057311
C	3.373911	4.794754	18.371316
C	4.015345	5.958837	17.977444
C	5.385527	6.134020	18.262516
C	3.449916	2.575005	19.472138
N	4.033460	1.600820	20.123041
C	5.372268	1.735951	20.438241
C	6.142494	2.887757	20.056591
C	7.498182	2.897293	20.397482
C	8.065069	1.829027	21.098490
C	7.196818	0.743730	21.462791
N	5.897275	0.709862	21.127270
N	7.636932	-0.346101	22.190045
C	8.898928	-0.392555	22.533950
C	9.878701	0.605174	22.209863
C	9.463412	1.753722	21.477243
C	11.224771	0.460855	22.612584
C	12.152877	1.439992	22.293203
C	11.746956	2.579068	21.566761
C	10.426392	2.737082	21.164577
H	9.220791	-1.264440	23.115704
H	8.119815	3.747211	20.115151
H	2.388799	2.440980	19.229476
H	2.313505	4.638541	18.159785
H	3.465442	6.739191	17.448820
H	5.887334	7.052534	17.952179
H	7.164198	5.319583	19.141910
H	11.517747	-0.428980	23.174575
H	13.194452	1.333414	22.600636
H	10.142912	3.627361	20.602407
H	12.480363	3.347763	21.315982
N	5.548368	-1.781059	23.804853
C	4.498200	-2.326449	23.069133
N	4.217611	-1.640189	21.907256
C	3.174685	-2.008464	21.082861
C	2.376339	-3.088039	21.385839
C	2.642371	-3.870203	22.586118
C	3.732806	-3.410709	23.445207
C	1.250640	-3.468961	20.462783
N	3.057988	-1.250093	19.923195
C	4.003406	-4.163861	24.718937
N	1.895618	-4.934900	22.840418
H	4.807264	-0.829259	21.641150

H	6.272668	-1.319254	23.230581
H	5.961645	-2.433572	24.465389
H	2.159336	-1.360159	19.459174
H	3.335716	-0.260186	20.019455
H	2.203500	-5.371105	23.717351
H	3.069313	-4.294971	25.293517
H	4.398007	-5.178094	24.524476
H	4.710534	-3.650981	25.386137
H	0.654046	-4.261041	20.934775
H	0.585226	-2.612837	20.245902
H	1.617028	-3.850560	19.492362

AAAA-DDDD, cation, Leigh (**X-11**)

N	-1.636518	14.828946	18.555996
C	-1.870216	13.920762	17.542866
C	-2.750687	12.789700	17.756785
C	-3.405837	12.633422	19.046718
C	-3.117287	13.604670	20.045325
C	-2.221713	14.665985	19.718637
C	-2.907014	11.905468	16.702753
C	-2.243083	12.134998	15.485893
C	-1.405627	13.306308	15.353795
N	-1.230947	14.168472	16.387803
C	-3.712748	13.505145	21.318183
C	-4.584580	12.463876	21.598335
C	-4.893688	11.489163	20.620829
C	-4.293804	11.592902	19.359362
N	-0.763822	13.587358	14.191843
C	-0.912853	12.742456	13.157564
C	-1.707437	11.531270	13.206993
C	-2.368956	11.260785	14.394134
N	-0.249127	13.097485	12.001707
C	-0.330338	12.323189	10.945291
C	-1.063911	11.101965	10.877614
C	-1.776459	10.679356	12.030902
C	-1.089536	10.316814	9.703635
C	-1.807071	9.135926	9.680640
C	-2.528397	8.690820	10.819288
C	-2.500605	9.472753	11.975216
C	-5.859124	10.335040	20.895351
C	-7.035367	10.418537	19.898487
C	-3.302337	7.376541	10.738192
C	-4.338357	7.473184	9.597763
C	-5.116343	8.997413	20.690961
C	-6.425547	10.367383	22.321774
C	-2.312081	6.232789	10.427810
C	-4.040879	7.042492	12.041409
H	-1.995312	15.413639	20.488858
H	-3.480015	14.255938	22.076663
H	-5.036717	12.401976	22.587385
H	-4.533565	10.840844	18.606727
H	-3.539392	11.020331	16.792582
H	-2.996211	10.374441	14.505443
H	-3.049814	9.136159	12.853263
H	-1.819416	8.533137	8.771584
H	-0.537036	10.653315	8.823500
H	0.215989	12.654908	10.053789
H	-7.113105	9.518941	22.451895
H	-6.988490	11.294310	22.511420
H	-5.628452	10.278300	23.076187
H	-6.685956	10.343799	18.857734
H	-7.581503	11.366772	20.016379
H	-7.732490	9.588102	20.087707
H	-4.732600	8.903260	19.664100
H	-5.809804	8.162678	20.875889
H	-4.270463	8.910080	21.389664
H	-4.781296	7.816844	12.295770
H	-3.341972	6.929584	12.885087
H	-4.575323	6.089377	11.915149
H	-5.061576	8.279194	9.794469
H	-4.885957	6.520897	9.524586
H	-3.856053	7.665956	8.628227
H	-1.563653	6.135161	11.229327
H	-1.786474	6.402163	9.476542
H	-2.866100	5.284579	10.350346
C	2.267698	15.181647	9.312226
C	2.135245	15.685190	10.608140
C	2.857179	16.825236	11.057686
C	3.741465	17.483759	10.194133
C	3.879087	16.980688	8.898108
C	3.154618	15.850731	8.463638
N	2.531408	17.093671	12.382615
C	1.654568	16.146712	12.700093
N	1.369358	15.281236	11.689126
N	1.041743	15.985421	13.938751
C	1.263059	16.819960	14.991661
N	2.081339	17.852949	14.890931
N	0.605221	16.546897	16.152110
C	0.752704	17.309589	17.306384
N	0.063892	16.972121	18.430867
C	0.422175	17.899782	19.395489
C	1.343528	18.775592	18.757106
N	1.531568	18.378053	17.438233
C	0.046973	18.058534	20.731573
C	0.622082	19.127627	21.425200
C	1.536692	20.003656	20.803126
C	1.909123	19.842456	19.466379
H	0.723548	14.444237	11.788078
H	0.393683	15.171362	14.055931
H	4.303083	18.357606	10.529129
H	4.563081	17.471589	8.203429
H	3.289738	15.490931	7.442179
H	1.707378	14.308811	8.970745
H	2.204131	18.434816	15.741445
H	2.554230	17.985651	13.976888
H	-0.032538	15.717914	16.197298
H	-0.600302	16.146511	18.494369
H	-0.659501	17.383618	21.219129
H	0.357937	19.287552	22.472022
H	1.961748	20.825934	21.381592
H	2.616716	20.519855	18.985213

AAAA-DDDD, cation, 2CH-N, Leigh (**X-13**)

C	1.444828	17.964748	20.655163
C	0.778273	16.730438	20.522992
C	0.447368	15.999789	21.695180
C	0.777673	16.523684	22.963745
C	1.427349	17.740207	23.063081
C	1.778277	18.483961	21.907004
C	-0.216051	14.736417	21.557155
N	-0.562788	14.176317	20.423880
C	-0.270953	14.855215	19.259375
C	0.400371	16.141644	19.248522
C	0.627836	16.736317	18.012676
C	0.225739	16.090477	16.827668
C	-0.423546	14.807911	16.939268
N	-0.664008	14.235024	18.138454
N	-0.825884	14.110445	15.853202
C	-0.639356	14.632586	14.633928
C	-0.017164	15.926029	14.419803
C	0.412882	16.627187	15.539051
N	-1.083475	13.840063	13.594467
C	-0.940606	14.296684	12.374845
C	-0.357763	15.557474	12.017157
C	0.125819	16.404621	13.053208
C	0.701743	17.635836	12.703305
C	0.811979	18.047379	11.369516
C	0.322943	17.189091	10.357730
C	-0.251390	15.966121	10.673876
C	1.454089	19.400256	11.056420
C	2.899066	19.407263	11.598899
C	2.504176	19.817516	22.076796
C	3.828869	19.575246	22.831579
C	1.496165	19.697909	9.551285
C	0.645962	20.515813	11.752971
C	2.823090	20.493477	20.736920
C	1.615370	20.767830	22.907655
N	-2.505042	12.106700	18.271120
C	-2.439679	11.127010	17.338424
N	-1.712000	11.405478	16.228351
C	-1.420216	10.508087	15.205161
C	-0.573769	10.717987	14.126867
N	-0.640522	9.551855	13.436287
N	-1.466678	8.669087	14.026989
N	-1.945889	9.252102	15.112128
C	-0.011141	9.246444	12.152357
C	-0.644633	10.038312	11.007820
C	0.017005	9.717956	9.667921
C	-0.612420	10.486339	8.503075
C	0.055314	10.166932	7.164307
C	-3.271871	12.071962	19.431213
N	-3.876926	10.954441	19.928421
N	-4.485871	11.268181	21.059980
N	-4.264294	12.578517	21.277820
C	-3.519196	13.131690	20.289550
C	-4.727988	13.233356	22.501240
C	-3.554973	13.771796	23.321482
C	-4.021580	14.469148	24.598776
C	-2.855324	15.045946	25.406718
C	-3.320101	15.749112	26.683680
N	-3.061656	9.961238	17.499006
H	-3.213965	14.169126	20.282970
H	-1.810499	12.904814	18.200437
H	-2.984769	9.263463	16.748358
H	-3.536302	9.784946	18.392746
H	-1.392119	12.400863	16.083931
H	0.003732	11.575237	13.806785
H	-1.301299	13.649965	11.564448
H	-0.628776	15.310981	9.884966
H	0.394953	17.487252	9.312225
H	1.075636	18.297860	13.485240
H	0.898995	17.600027	15.443088
H	1.116030	17.710053	17.938446
H	1.709987	18.526593	19.760462
H	1.678114	18.134845	24.048784
H	0.517970	15.955131	23.860159
H	-0.456590	14.179601	22.471506
H	1.966944	20.679600	9.394504
H	0.484648	19.731852	9.117556
H	2.087032	18.945667	9.006066
H	0.624678	20.376639	12.844109
H	-0.390829	20.535129	11.383907
H	1.111229	21.490734	11.540339
H	2.920544	19.249595	12.687611
H	3.366225	20.381156	11.384410
H	3.499636	18.618495	11.120609
H	1.906448	20.720665	20.170065
H	3.477925	19.864952	20.113313
H	3.346133	21.441868	20.929662
H	0.664441	20.965893	22.389267
H	2.140875	21.724388	23.053303
H	1.390664	20.345366	23.898195
H	4.486972	18.902249	22.260730
H	3.653545	19.132823	23.823401
H	4.347858	20.536052	22.972067
H	-0.133415	8.165489	12.001028
H	1.062827	9.468593	12.238607
H	-1.720830	9.803858	10.963798
H	-0.553089	11.118068	11.217287
H	1.094785	9.953698	9.721980
H	-0.058987	8.633893	9.470791
H	-1.687964	10.244154	8.453321
H	-0.543917	11.569975	8.706233
H	-0.413205	10.720722	6.336354
H	1.124901	10.431133	7.188039
H	-0.019243	9.090971	6.938650
H	-5.291800	12.474077	23.059178
H	-5.415992	14.045359	22.221650
H	-2.878682	12.937359	23.570635
H	-2.980168	14.484287	22.706278
H	-4.722856	15.281999	24.340174
H	-4.583148	13.755371	25.226429
H	-2.155481	14.231182	25.661198
H	-2.295033	15.755333	24.772019
H	-2.470529	16.154971	27.253776

H	-3.999996	16.582574	26.444711
H	-3.864948	15.049365	27.337585

AAAA-DDDD, cation, model (**X-15**)

H	2.943708	15.185635	9.105910
C	2.534584	15.433428	10.099871
N	2.819898	16.526807	10.720104
C	3.672926	17.402847	10.072910
N	4.043325	18.483510	10.686914
C	4.919081	19.286550	9.983277
N	5.415672	20.338249	10.547575
C	6.319161	21.063074	9.766345
N	6.908696	22.074999	10.274545
C	7.857863	22.806213	9.459011
H	4.020129	17.152564	9.050847
H	5.186478	18.996256	8.948833
H	6.501357	20.724259	8.727010
H	1.859410	14.717915	10.579003
H	7.547871	23.862258	9.414182
H	8.841228	22.786613	9.956068
H	7.958596	22.406034	8.434303
N	6.084119	22.981011	12.863563
H	6.623946	23.786437	13.163681
C	5.321721	22.378215	13.809063
N	4.688186	21.192619	13.355090
C	3.809187	20.453528	14.098538
N	3.247378	19.356398	13.498736
C	2.277647	18.519544	14.102173
N	1.771391	17.578630	13.256273
H	1.177081	16.875631	13.685001
N	5.110826	22.793121	15.022732
N	3.509583	20.785367	15.334611
N	1.921059	18.725591	15.332281
H	2.244482	17.282402	12.388806
H	3.523592	19.129908	12.527123
H	3.992721	21.652878	15.676624
H	2.815708	20.155830	15.799991
H	4.901295	20.882597	12.386933
H	6.350480	22.557282	11.949749
H	5.622236	23.656678	15.219311
H	1.210649	18.055191	15.636098

AAAA-DDDD, neutral, Leigh (**X-12**)

C	2.602769	15.019001	9.535724
C	2.380810	15.540344	10.825823
C	3.088314	16.703952	11.223263
C	3.992841	17.317982	10.330625
C	4.192205	16.781940	9.072256
C	3.498893	15.618149	8.650151
C	1.466824	14.953962	11.792534
C	1.339702	15.563457	13.103125
N	2.057274	16.698662	13.425547
C	2.865061	17.220291	12.537738
C	0.693154	13.831649	11.541713
C	-0.156331	13.326024	12.540256
C	-0.198522	13.993183	13.824836
N	0.545155	15.098378	14.076741
N	-0.985908	13.539983	14.832613
C	-1.739948	12.454997	14.611139
C	-1.778844	11.729358	13.356056
C	-0.964397	12.193384	12.335873
C	-2.649880	10.568634	13.236913
C	-3.407771	10.203355	14.383405
C	-3.277332	10.996704	15.566597
N	-2.508218	12.048606	15.686279
C	-4.263489	9.086094	14.334130
C	-4.372653	8.342254	13.168487
C	-3.635812	8.688208	12.012487
C	-2.784561	9.798469	12.070525
C	-3.743523	7.895496	10.707608
C	-4.711083	6.708836	10.819505
C	3.767132	15.062706	7.252117
C	2.930614	13.814752	6.940754
C	-4.247763	8.833569	9.590171
C	-2.349344	7.354723	10.324643
C	3.437839	16.148750	6.205425
C	5.262321	14.692935	7.142628
H	-3.862707	10.714261	16.450085
H	-4.839009	8.814044	15.222045
H	-5.040073	7.481533	13.148698
H	-2.216858	10.067691	11.179191
H	-0.930654	11.695393	11.365188
H	0.728018	13.322137	10.577219
H	2.067063	14.124264	9.221914
H	4.897478	17.261447	8.391583
H	4.531028	18.214030	10.648346
H	3.411735	18.121305	12.842149
H	-4.746420	6.183614	9.853783
H	-5.731934	7.041004	11.063146
H	-4.383549	5.990449	11.586650
H	-3.560488	9.678240	9.433959
H	-5.242526	9.235078	9.837907
H	-4.323029	8.270889	8.646358
H	-1.625533	8.170793	10.180951
H	-2.422339	6.791029	9.381544
H	-1.963722	6.681064	11.105248
H	1.851725	14.031844	6.983073
H	3.153349	12.994924	7.641587
H	3.168720	13.467300	5.924493
H	2.374581	16.429596	6.254564
H	3.651346	15.760716	5.197260
H	4.044410	17.053293	6.358940
H	5.526242	13.912935	7.873215
H	5.906542	15.566966	7.319713
H	5.471162	14.311820	6.130890
N	-2.446628	13.220223	18.207591
C	-1.756714	14.325965	18.641543
N	-1.960682	14.614437	19.925281
C	-2.841675	13.635074	20.364823
C	-3.158574	12.748927	19.296881
C	-3.406889	13.433775	21.630282
C	-4.275818	12.349293	21.798363
C	-4.580508	11.479640	20.732277
C	-4.025003	11.666589	19.459633
N	-0.948152	15.015582	17.765685
C	-0.204990	16.163988	18.131725
N	-0.173877	16.714427	19.285370
N	0.523149	16.650879	17.037000
C	1.356863	17.753918	17.043221
N	1.600605	18.603108	18.031159
C	2.506263	19.504264	17.487610
C	2.796050	19.168567	16.133626
N	2.041466	18.040500	15.878243
C	3.123630	20.617269	18.074386
C	4.013095	21.367314	17.295706
C	4.287990	21.023330	15.956565
C	3.681225	19.914159	15.351903
H	1.997351	17.497871	14.981872
H	0.481576	16.134829	16.150056
H	2.912257	20.882292	19.112621
H	4.506458	22.237390	17.733792
H	4.986797	21.630879	15.377976
H	3.900033	19.654534	14.313568
H	-0.786341	16.184352	19.922146
H	-0.906858	14.650180	16.804033
H	-2.437691	12.823186	17.232717
H	-4.263678	10.987088	18.638459
H	-5.262734	10.643886	20.899915
H	-4.727161	12.171430	22.776755
H	-3.172090	14.107416	22.456880

AAAA-DDDD, neutral, 2CH-N, Leigh (**X-14**)

N	-2.974185	14.043763	21.774260
C	-3.013989	12.912044	21.000433
C	-3.772494	11.951381	21.660262
N	-4.148587	12.573780	22.814097
N	-3.674385	13.830565	22.877391
N	-2.365353	12.898144	19.784117
C	-2.213080	11.776057	18.981926
N	-2.705892	10.628458	19.315726
C	-5.039556	12.062374	23.849578
N	-1.474323	12.082593	17.832408
C	-1.189672	11.196479	16.804946
C	-0.722426	11.528790	15.538268
N	-0.562215	10.326039	14.929700
N	-0.916152	9.307018	15.734414
N	-1.297740	9.835112	16.891301
C	-0.095546	10.093731	13.566268
C	-1.056541	10.664319	12.523502
C	-0.439107	10.638923	11.125214
C	-1.373684	11.210806	10.057397
C	-0.695832	11.334221	8.690860
N	-0.130489	14.009148	12.566621
C	0.244721	14.297104	11.348199
C	0.906659	15.505334	10.937240
C	1.209298	16.485463	11.921626
C	0.830407	16.183301	13.293297
C	0.136017	14.937108	13.562721
C	1.247703	15.739601	9.591876
C	1.874758	16.921954	9.222280
C	2.183261	17.912261	10.182950
C	1.844630	17.671634	11.519135
C	1.085528	17.015418	14.374562
C	0.659034	16.649892	15.666215
C	-0.055474	15.402213	15.825065
N	-0.290831	14.584001	14.776858
N	-0.529224	14.997177	17.029764
C	-0.317939	15.777780	18.094389
C	0.423322	17.024786	18.046594
C	0.890719	17.439676	16.806944
C	0.619737	17.765978	19.281621
C	0.023391	17.239266	20.456880
C	-0.718505	16.015269	20.368638
N	-0.875054	15.314653	19.272188
C	0.175121	17.919220	21.684526
C	0.910697	19.089332	21.742871
C	1.522036	19.631905	20.583517
C	1.362751	18.960490	19.371291
C	2.870894	19.229077	9.812785
C	3.159436	19.340476	8.309359
C	2.334336	20.921211	20.706847
C	2.926341	21.377048	19.366245
C	1.421754	22.042575	21.246885
C	3.493202	20.689270	21.699602
C	1.963578	20.407831	10.224893
C	4.207956	19.329724	10.577238
H	-4.031185	10.934644	21.400381
H	-1.852164	13.771090	19.536070
H	-2.468455	9.932230	18.599732
H	-1.264344	13.069364	17.618808
H	-0.524424	12.490809	15.066691
H	0.025411	13.547022	10.577198
H	1.009316	14.981461	8.841287
H	2.127650	17.083699	8.174856
H	2.077139	18.435217	12.262868
H	1.618422	17.960455	14.248452
H	1.438226	18.377782	16.694474
H	1.829043	19.366429	18.474479
H	1.024804	19.603203	22.698535
H	-0.291721	17.506395	22.581804
H	-1.213957	15.614704	21.263050
H	3.649306	20.305222	8.109170
H	2.232685	19.298260	7.716759
H	3.832504	18.539246	7.967133
H	1.766376	20.403517	11.307140
H	0.999618	20.361626	9.695836
H	2.458250	21.358155	9.970107
H	4.048920	19.304182	11.665406
H	4.706459	20.278865	10.324055
H	4.877254	18.499999	10.303157
H	2.137579	21.581659	18.625576
H	3.612814	20.622341	18.951367
H	3.495854	22.305215	19.522185
H	0.589071	22.235636	20.553260
H	2.006497	22.969205	21.358176

H	1.002606	21.780661	22.229560
H	4.163312	19.894106	21.337629
H	3.119295	20.402507	22.693468
H	4.076239	21.617567	21.805477
H	0.023727	9.006866	13.459868
H	0.895011	10.564455	13.464184
H	-1.999214	10.093226	12.542599
H	-1.280720	11.710615	12.784289
H	0.495525	11.228461	11.142315
H	-0.154009	9.608045	10.848494
H	-2.269067	10.571518	9.976710
H	-1.732810	12.200750	10.389434
H	-1.381425	11.739551	7.931161
H	0.181750	12.000957	8.747321
H	-0.339625	10.352378	8.339926
C	-6.501758	12.052996	23.400150
H	-4.707355	11.047719	24.116428
H	-4.903575	12.714606	24.723478
C	-7.429403	11.548151	24.505975
H	-6.789986	13.075663	23.105185
H	-6.602858	11.414377	22.507017
C	-8.897479	11.512957	24.074153
H	-7.116813	10.534768	24.815908
H	-7.326495	12.194569	25.396061
C	-9.826770	11.026222	25.188360
H	-9.201061	12.522968	23.748303
H	-8.995847	10.857104	23.192002
H	-10.876449	11.002013	24.857021
H	-9.549365	10.009961	25.512595
H	-9.762816	11.687740	26.067939

AAAA-DDDD, neutral, model (**X-16**)

C	1.819125	15.890878	9.064685
N	1.746609	15.991853	10.346137
C	2.471493	17.021525	10.930754
N	2.326395	17.235190	12.197869
C	3.094780	18.248029	12.740411
N	2.932084	18.555624	13.983842
C	3.736670	19.572143	14.492159
N	3.557162	19.958016	15.698145
C	4.402787	21.019560	16.204861
H	2.401573	16.589750	8.439123
H	3.156338	17.619486	10.294856
H	3.834057	18.763792	12.094294
H	4.510145	20.015295	13.829461
H	1.275344	15.079760	8.570296
H	4.932769	20.654700	17.099530
H	5.139832	21.394109	15.469455
H	3.764892	21.854873	16.537631
N	0.857095	19.231743	16.868880
C	0.034299	18.211785	16.417319
N	-1.224267	18.075565	16.683059
N	0.708927	17.296167	15.602213
C	0.442151	15.920302	15.525980
N	-0.032936	15.246759	16.504870
N	0.806363	15.427463	14.252560
C	0.716711	14.103858	13.830157
N	0.509039	13.138391	14.674393
N	0.807672	13.960843	12.457282
H	0.384879	20.100604	17.101990
H	1.061926	13.034159	12.129320
H	1.116164	14.733417	11.856989
H	1.099406	16.114883	13.550339
H	-0.126363	14.265337	16.198657
H	1.513471	17.658723	15.070360
H	1.806135	19.347003	16.485226
H	-1.509587	18.807964	17.344121
H	0.413215	12.250123	14.171116

Molecules optimized at CPCM/M06-2X/6-31-G** level of theory using Gaussian 09

AA-DD Np

C	-3.528425	0.051293	0.435646
C	-2.146122	-0.040928	0.561225
C	-1.594303	-0.198800	1.834272
C	-2.399826	-0.266006	2.969509
C	-3.782400	-0.174557	2.853318
C	-4.314103	-0.017465	1.578961
C	-1.246852	0.030633	-0.671726
C	-0.473643	-1.259988	-0.857099
C	0.880645	-1.312670	-0.630825
N	1.587648	-0.173982	-0.326065
C	1.029577	1.085765	-0.382015
C	-0.324929	1.232117	-0.609052
N	1.641318	-2.446436	-0.645236
C	-1.184844	-2.458471	-1.243975
O	-2.497213	-2.216643	-1.445059
C	-3.318035	-3.346353	-1.759710
C	-4.744606	-2.845594	-1.832176
C	-0.884028	2.553938	-0.727073
O	-2.217028	2.516565	-0.959145
C	-2.890824	3.776123	-1.024376
C	-4.368049	3.477401	-1.167680
N	1.905798	2.089022	-0.184879
N	-5.770053	0.081025	1.432445
O	-6.452876	0.047242	2.442160
O	-0.717594	-3.587549	-1.385552
O	-0.287849	3.627821	-0.635460
O	-6.226867	0.192206	0.305731
N	4.879291	1.248481	-0.271372
C	5.307229	0.059158	0.231124
C	6.672306	-0.198329	0.512753
C	7.613036	0.826099	0.243116
C	7.168995	2.014637	-0.269990
C	5.781194	2.175627	-0.505585
N	4.340127	-0.871826	0.450638
C	4.692871	-2.033406	0.955637
C	6.026572	-2.381316	1.279255
C	7.016075	-1.462645	1.051441
H	6.239769	-3.359279	1.693440
H	7.848191	2.828587	-0.492840
H	5.411537	3.117955	-0.903406
H	3.889511	-2.749578	1.118371
H	2.566815	-0.286825	-0.035891
H	-1.917444	0.153193	-1.528600
H	2.901283	1.894788	-0.262126
H	1.540618	3.025096	-0.304492
H	-2.674958	4.345866	-0.115590
H	-2.505937	4.349010	-1.874140
H	-4.936909	4.408843	-1.213431
H	-4.558416	2.909126	-2.081521
H	-4.725931	2.890927	-0.317178
H	1.156283	-3.259943	-1.009170
H	2.604886	-2.326816	-0.927531
H	-2.986702	-3.778783	-2.708881
H	-3.189070	-4.107550	-0.984676
H	-5.420805	-3.672837	-2.059542
H	-5.045588	-2.399502	-0.880439
H	-4.846931	-2.088706	-2.613674
H	-0.512984	-0.268286	1.931484
H	-1.951208	-0.389633	3.949122
H	-4.437113	-0.221588	3.713888
H	-3.988509	0.176261	-0.537994
H	8.665289	0.652264	0.447963
H	8.055781	-1.681293	1.276895

AAA-DDD, cation, Leigh

C	3.677745	-2.694812	0.126958
C	2.284995	-2.506651	0.079197
C	1.449407	-3.642329	0.085705
C	1.997746	-4.936995	0.137951
C	3.365979	-5.100783	0.185313
C	4.203407	-3.971804	0.179330
C	0.025744	-3.445744	0.028028
N	-0.564006	-2.292421	-0.007897
C	0.216751	-1.150548	0.007084
C	1.638248	-1.205851	0.029239
C	2.324507	0.004623	-0.001337
C	1.632312	1.211739	-0.031855
C	0.211148	1.149528	-0.009847
N	-0.464580	-0.002145	-0.001547
N	-0.575129	2.287610	0.005771
C	0.009075	3.443800	-0.028195
C	1.431802	3.647358	-0.084869
C	2.272801	2.515685	-0.080458
C	3.664626	2.710609	-0.128347
C	4.184123	3.990223	-0.178131
C	3.341332	5.115190	-0.181277
C	1.973893	4.944757	-0.134274
N	-3.386613	2.159670	0.787836
C	-4.150060	1.127276	0.401685
N	-3.500561	-0.005894	-0.000178
C	-4.144591	-1.142346	-0.401481
C	-5.541875	-1.153784	-0.409983
C	-6.215223	-0.012804	0.001089
C	-5.547312	1.131665	0.411396
N	-3.376451	-2.171077	-0.787804
H	-0.614766	-4.327469	0.010029
H	1.333396	-5.795895	0.141275
H	3.797934	-6.094334	0.227962
H	5.279449	-4.104024	0.217646
H	4.351519	-1.845958	0.126874
H	3.407880	0.007339	-0.001038
H	4.342452	1.864979	-0.130407
H	5.259504	4.127669	-0.216498
H	3.768540	6.110889	-0.221460
H	1.305368	5.800430	-0.135600
H	-0.635704	4.322404	-0.009318
H	-2.464510	-0.003478	-0.000681
H	-2.381960	-2.204120	-0.532349
H	-3.836162	-3.043371	-0.996785
H	-6.063930	-2.047857	-0.722990
H	-7.300479	-0.015638	0.001773
H	-6.073616	2.023007	0.725008
H	-2.392677	2.196827	0.531034
H	-3.850344	3.030387	0.994717

AAA-DDD, neutral, Leigh

C	-5.724500	-0.130368	0.215814
C	-4.968375	-1.299344	0.215167
C	-3.566917	-1.170033	0.003100
N	-2.964550	0.007397	-0.171689
C	-3.703930	1.117948	-0.161333
C	-5.115789	1.106569	0.023172
C	-5.523328	-2.628368	0.412919
C	-4.625370	-3.713984	0.371041
C	-3.231038	-3.443322	0.131303
N	-2.722501	-2.265904	-0.040057
N	0.031127	-2.041596	-1.213689
C	0.830844	-1.001540	-0.912123
N	0.172692	0.108564	-0.418277
C	0.797853	1.331891	-0.269738
C	2.166270	1.440185	-0.433866
C	3.030759	0.222148	-0.681505
C	2.201439	-0.977291	-1.091323
C	3.886595	-0.096389	0.544917
C	5.275059	-0.054911	0.469283
C	6.020619	-0.347183	1.604117
C	5.442826	-0.681932	2.822915
C	4.054617	-0.720916	2.889794
C	3.289047	-0.431308	1.761425
N	7.483061	-0.300488	1.510013
O	7.980008	-0.000047	0.435864
C	2.794713	2.729987	-0.311954
O	2.254254	3.808300	-0.059132
N	-0.021240	2.347318	0.060672
C	2.870271	-2.152084	-1.587469
O	2.362842	-3.234816	-1.885937
O	4.132164	2.657828	-0.510317
C	4.872173	3.867946	-0.336306
C	6.334615	3.515583	-0.507246
O	4.205594	-1.959536	-1.704588
C	4.980633	-3.088745	-2.114396
C	6.428641	-2.646782	-2.127413

O	8.132329	-0.564430	2.508130
C	-5.830796	2.372501	0.003805
C	-5.082958	-5.031645	0.552459
H	-2.543884	-4.288761	0.086929
N	-2.992299	2.290594	-0.345469
H	-0.847349	0.074871	-0.346816
H	3.733957	0.451713	-1.489310
H	-0.913318	-2.078217	-0.831645
H	0.512749	-2.895835	-1.466095
H	4.812072	-3.912437	-1.413530
H	4.645040	-3.420426	-3.101900
H	7.072159	-3.478895	-2.422278
H	6.572880	-1.827855	-2.836514
H	6.735832	-2.301434	-1.136556
H	0.417700	3.259750	0.092880
H	4.539977	4.605476	-1.073839
H	4.664516	4.276888	0.657296
H	6.953980	4.405652	-0.374334
H	6.637983	2.765243	0.228021
H	6.517318	3.110485	-1.505680
H	2.203193	-0.464667	1.819208
H	3.569758	-0.977851	3.825351
H	6.067537	-0.902190	3.678948
H	5.770706	0.200206	-0.460615
C	-6.886303	-2.890398	0.642821
H	-6.796409	-0.183929	0.365512
C	-3.641971	3.409548	-0.360682
H	-1.024392	2.269762	-0.105426
H	-3.056788	4.318406	-0.504380
C	-5.067224	3.539767	-0.198524
C	-5.682864	4.803844	-0.230784
C	-7.047566	4.907650	-0.062478
H	-5.071470	5.687713	-0.387958
H	-7.530723	5.878162	-0.085971
C	-7.814007	3.747163	0.140518
C	-7.221565	2.499030	0.173454
H	-8.887540	3.831382	0.273326
H	-7.841486	1.623830	0.332065
C	-6.422960	-5.268449	0.776106
H	-4.370455	-5.850388	0.513317
H	-6.785270	-6.280649	0.917146
C	-7.322541	-4.189527	0.820871
H	-7.605605	-2.080424	0.684823
H	-8.376042	-4.378601	0.998187

AAA-DDD, OH, Leigh

C	-3.304021	-1.063359	-0.643437
C	-4.458315	-0.267555	-0.618881
C	-5.411941	-0.484454	0.368643
C	-5.251693	-1.480693	1.336469
C	-4.077297	-2.231890	1.305931
C	-3.086456	-2.035010	0.342260
C	-4.572674	0.826219	-1.652536
O	-3.533685	1.785668	-1.541246
C	-6.320948	-1.745885	2.366547
C	-1.777485	-2.785683	0.432771
O	-1.248504	-3.065734	-0.854599
O	-2.428384	-0.818728	-1.650927
N	1.439182	-2.436726	-0.463381
C	1.539893	-1.061422	-0.296872
C	2.780496	-0.428248	-0.008628
C	3.978382	-1.246232	0.084504
C	3.827456	-2.635541	-0.101884
C	2.510623	-3.155229	-0.367529
N	0.390792	-0.400751	-0.424788
C	0.387468	0.922947	-0.258831
C	1.566660	1.661956	0.056764
C	2.758650	0.952699	0.170133
C	1.461197	3.100659	0.242007
C	0.183487	3.675655	0.093005
C	-0.923861	2.812823	-0.241055
N	-0.847297	1.532854	-0.410789
C	2.545302	3.939847	0.558909
C	2.349147	5.298392	0.718028
C	1.072512	5.866896	0.568021
C	-0.002314	5.059722	0.257516
C	4.939345	-3.494414	-0.030153
C	6.192336	-2.977478	0.223015
C	6.348921	-1.592976	0.408850
C	5.265121	-0.738508	0.341997
H	-3.917683	-2.997177	2.064125
H	-6.303885	0.139284	0.383711
H	-1.911500	3.257925	-0.372354
H	3.677489	1.478472	0.402182
H	2.398534	-4.231142	-0.500787
H	4.795023	-4.560784	-0.177497
H	7.055085	-3.631999	0.277392
H	7.335839	-1.187275	0.605629
H	5.420043	0.324654	0.486547
H	-0.997299	5.477779	0.135870
H	0.937117	6.935241	0.696398
H	3.542311	3.532274	0.681702
H	3.193674	5.934079	0.962912
H	-0.272444	-2.964350	-0.784917
H	-1.675733	-1.433608	-1.543718
H	-2.694923	1.294381	-1.498148
H	-6.864934	-0.831291	2.616440
H	-7.054180	-2.472276	1.999369
H	-5.892959	-2.150128	3.287478
H	-1.933387	-3.715809	0.996680
H	-1.058179	-2.173725	0.996461
H	-5.519075	1.360293	-1.524696
H	-4.573044	0.378483	-2.657282

AAA-DDD, cation, model

C	6.447950	3.983324	-0.005562
C	5.924499	2.704382	-0.003879
C	4.531456	2.512038	-0.002915
C	3.693494	3.646021	-0.003707
C	4.239397	4.942724	-0.005388
C	5.607987	5.110439	-0.006323
C	2.269564	3.444995	-0.002797
N	1.684801	2.288970	-0.001572
C	2.466172	1.148376	-0.000961
C	3.887744	1.208607	-0.001261
N	1.784652	0.000004	-0.000076
C	2.466170	-1.148369	0.000882
C	3.887742	-1.208604	0.001329
C	4.577554	0.000001	0.000070
C	4.531451	-2.512038	0.003033
C	3.693488	-3.646019	0.003712
C	2.269558	-3.444988	0.002673
N	1.684797	-2.288962	0.001414
C	4.239385	-4.942725	0.005411
C	5.607974	-5.110445	0.006485
C	6.447939	-3.983333	0.005849
C	5.924492	-2.704388	0.004144
N	-1.188900	-2.264610	-0.002628
C	-1.980600	-1.207676	-0.001734
N	-1.342332	-0.000022	-0.000301
C	-1.980590	1.207638	0.001244
C	-3.398347	1.248028	0.001758
C	-4.118441	-0.000012	-0.000331
C	-3.398351	-1.248052	-0.002217
N	-1.188867	2.264559	0.002094
C	-4.014462	-2.582949	-0.004221
O	-5.357767	-2.598223	-0.005299
C	-5.984529	-3.899146	-0.006963
C	-7.478346	-3.668515	-0.007585
N	-5.447724	-0.000017	-0.000511
C	-4.014454	2.582931	0.004162
O	-5.357766	2.598235	0.005323
C	-5.984476	3.899182	0.007789
C	-7.478297	3.668626	0.008200
O	-3.395741	-3.638054	-0.005062
O	-3.395716	3.638037	0.005409
H	1.624752	4.323750	-0.003182
H	-0.311566	-0.000024	-0.000292
H	-0.160997	2.180441	0.001210
H	-1.640513	3.171550	0.003668
H	-5.647542	4.442138	0.893804
H	-5.648483	4.445098	-0.876752
H	-7.995475	4.630310	0.010252
H	-7.784614	3.113794	-0.881645
H	-7.783621	3.110555	0.896352
H	-1.640562	-3.171593	-0.003807
H	-5.647582	-4.442699	-0.892608
H	-5.648594	-4.444494	0.877958
H	-7.995591	-4.630164	-0.008872
H	-7.784637	-3.112951	0.881813
H	-7.783621	-3.111131	-0.896190
H	5.660866	-0.000001	0.000125
H	-0.161029	-2.180509	-0.001549
H	1.624745	-4.323742	0.002989
H	3.572780	-5.799901	0.005898
H	6.038108	-6.105711	0.007869
H	7.524259	-4.118648	0.006746
H	6.600319	-1.857178	0.003766
H	3.572794	5.799903	-0.005969
H	6.038126	6.105702	-0.007691
H	6.600323	1.857170	-0.003404
H	7.524271	4.118634	-0.006343
H	-5.947370	0.874746	0.000859
H	-5.947367	-0.874778	-0.002307

AAA-DDD, anion, model

C	-5.542703	3.258919	-0.289910
C	-4.165752	2.962491	-0.277639
C	-3.248341	4.025822	-0.408278
C	-3.701143	5.351192	-0.546735
C	-5.052991	5.619940	-0.556466
C	-5.973032	4.564165	-0.427066
C	-1.840778	3.725293	-0.389290
N	-1.345450	2.535133	-0.274384
C	-2.209859	1.463626	-0.158460
C	-3.621767	1.620782	-0.141478
C	-4.398936	0.473447	0.005313
C	-3.802657	-0.783478	0.119602
C	-2.372462	-0.817369	0.065652
N	-1.615282	0.268063	-0.062172
N	-1.665753	-2.012197	0.142426
C	-2.319184	-3.118781	0.277479
C	-3.761175	-3.228494	0.363863
C	-4.508049	-2.025086	0.278367
C	-4.394876	-4.441782	0.515571
C	-5.834584	-4.516363	0.594131
N	-6.547388	-3.312052	0.507089
C	-5.908959	-2.175067	0.361209
N	1.194550	-2.165264	-0.506174
C	2.073589	-1.164011	-0.412360
N	1.514575	0.079260	-0.246551
C	2.253203	1.200335	0.059449
C	3.644660	1.144714	0.022300
C	4.300162	-0.066736	-0.516466
C	3.466376	-1.294127	-0.490555
C	4.372938	2.329752	0.458879
O	5.670372	2.127094	0.734630
C	6.396758	3.273146	1.184733
C	7.834493	2.838081	1.370725
N	1.518858	2.268620	0.407237
C	4.004171	-2.640046	-0.549865
O	5.352391	-2.707948	-0.464494
C	5.917252	-4.023869	-0.492014
C	7.420870	-3.860313	-0.440988
N	5.493296	0.020146	-0.993435
O	3.351018	-3.680631	-0.634406
O	3.875001	3.442992	0.639302
H	-1.730094	-4.035995	0.327340
H	0.491826	0.143786	-0.191349
H	0.206124	-2.031277	-0.270306
H	1.590023	-3.092992	-0.595628
H	5.539443	-4.593265	0.362484
H	5.591659	-4.536479	-1.401760
H	7.902469	-4.840885	-0.451594
H	7.774655	-3.290071	-1.303386

H	7.719837	-3.334813	0.468795
H	2.035349	3.133584	0.501901
H	6.306654	4.072403	0.442857
H	5.957328	3.640508	2.117756
H	8.441857	3.683716	1.701982
H	7.903432	2.045452	2.119399
H	8.242096	2.460920	0.430054
H	-5.479479	0.554754	0.030559
H	0.517328	2.287315	0.204059
H	-1.134000	4.551214	-0.473950
H	-2.972074	6.150372	-0.645295
H	-5.409837	6.638500	-0.662995
H	-7.036974	4.777152	-0.435289
H	-6.276080	2.466376	-0.193556
H	-3.826523	-5.364836	0.579186
O	-6.448205	-5.588059	0.732801
H	-6.541606	-1.286373	0.304590
H	5.786777	-0.895723	-1.325002

AAA-DDD, neutral, model

C	-3.379951	1.174158	-0.554967
C	-1.992359	1.125587	-0.482691
N	-1.364754	-0.073473	-0.224347
C	-2.040398	-1.208277	0.147364
C	-3.436497	-1.245966	0.066771
C	-4.147393	-0.091268	-0.538718
N	-1.156442	2.161301	-0.658173
N	-1.255984	-2.204891	0.581245
C	-4.093969	-2.457955	0.524701
O	-3.534678	-3.484629	0.909722
N	-5.321537	-0.116757	-1.064829
C	-3.999246	2.491106	-0.646610
O	-3.405231	3.534798	-0.924153
O	-5.300893	2.524957	-0.327044
C	-5.923689	3.811245	-0.382682
C	-7.389163	3.604692	-0.065754
O	-5.442400	-2.387884	0.541636
C	-6.128006	-3.558029	1.005885
C	-7.610257	-3.276846	0.891173
N	1.689397	2.286145	0.242653
C	2.463933	1.143274	0.150671
C	3.886714	1.184956	0.179675
C	4.541412	2.472235	0.346055
C	3.712999	3.608131	0.447764
C	2.285888	3.426554	0.376460
C	4.563877	-0.023080	0.038197
C	3.860597	-1.216123	-0.103819
C	2.439542	-1.142411	-0.079123
N	1.773562	0.007803	0.032326
C	4.486820	-2.517135	-0.271288
C	3.633667	-3.634364	-0.376300
C	2.210948	-3.421747	-0.301932
N	1.639634	-2.268469	-0.166904
C	4.161807	-4.927423	-0.543952
C	5.527277	-5.108317	-0.609969
C	6.382325	-3.997604	-0.507639
C	5.876720	-2.722447	-0.340341
C	4.269300	4.889909	0.610690
C	5.638400	5.041342	0.675226
C	6.468985	3.911781	0.577177
C	5.935446	2.647367	0.414875
H	1.557000	-4.292170	-0.360739
H	-0.343094	-0.071978	-0.153411
H	-0.253241	-2.174956	0.396814
H	-1.722999	-3.083627	0.766086
H	-5.825652	-4.415721	0.398483
H	-5.828670	-3.760000	2.038510
H	-8.180189	-4.140619	1.240970
H	-7.885494	-2.409574	1.495430
H	-7.884549	-3.077808	-0.147631
H	-1.604953	3.055956	-0.813300
H	-5.440854	4.480455	0.336754
H	-5.779424	4.240131	-1.378794
H	-7.918498	4.559547	-0.105149
H	-7.841976	2.922858	-0.789150
H	-7.511290	3.179648	0.933162
H	5.647534	-0.034921	0.038785
H	-0.197835	2.120243	-0.311658
H	1.651560	4.311107	0.437719
H	3.608645	5.748703	0.684120
H	6.076146	6.025266	0.801679
H	7.545783	4.033261	0.630525
H	6.603824	1.796748	0.346545
H	3.482562	-5.771292	-0.620696
H	5.943706	-6.100905	-0.740487
H	6.563637	-1.887005	-0.268828
H	7.456188	-4.142391	-0.561749
H	-5.713764	-1.050590	-0.970489

AAA-DDD, wd ester, model

C	4.392994	-2.667907	-0.244297
C	2.998854	-2.487405	-0.193296
C	2.168127	-3.624738	-0.249050
C	2.723283	-4.913219	-0.350660
C	4.092574	-5.070123	-0.399127
C	4.925290	-3.939085	-0.345806
C	0.740127	-3.437186	-0.194611
N	0.142109	-2.292367	-0.117093
C	0.922216	-1.148885	-0.073724
C	2.345150	-1.193120	-0.090739
C	3.022845	0.019956	-0.002510
C	2.321463	1.219922	0.080507
C	0.900276	1.148045	0.051672
N	0.237254	-0.006592	-0.013633
N	0.097465	2.276107	0.087747
C	0.672266	3.432291	0.171891
C	2.095959	3.647376	0.240312
C	2.949018	2.526371	0.190415
C	2.625144	4.946117	0.350049
C	3.990633	5.129150	0.412581
C	4.845434	4.014528	0.365006
C	4.338907	2.733559	0.255336
H	0.021643	4.306896	0.190977
H	4.106507	0.030388	0.001744
H	0.106786	-4.324212	-0.219009
H	2.061953	-5.773716	-0.390640
H	4.528609	-6.059665	-0.479625
H	6.002144	-4.064919	-0.386139
H	5.062157	-1.815888	-0.209109
H	1.946976	5.793620	0.385748
H	4.406985	6.126580	0.499445
H	5.024651	1.894632	0.224869
H	5.919212	4.160976	0.416339
N	-2.706876	1.978544	-1.204166
C	-3.523392	1.028134	-0.602422
N	-2.830417	0.008573	0.000723
C	-3.481279	-1.042835	0.600635
C	-4.842545	-1.104160	0.642314
C	-5.636276	-0.043142	0.032159
C	-4.890784	1.026326	-0.631328
C	-5.524383	-2.259302	1.322573
N	-2.640945	-1.969232	1.200513
C	-5.666776	2.103922	-1.336329
N	-6.937941	-0.103495	0.099612
H	-1.807788	0.026410	0.002961
H	-1.796335	2.077354	-0.754847
H	-3.152995	2.879071	-1.304051
H	-3.098243	-2.851437	1.385851
H	-1.749901	-2.100723	0.721649
H	-7.343127	0.709932	-0.362840
H	-6.419906	1.657934	-1.996745
H	-6.204994	2.757104	-0.637760
H	-5.037319	2.734329	-1.967239
H	-6.600640	-2.090226	1.302472
H	-5.322300	-3.216272	0.822779
H	-5.209369	-2.366459	2.367955

AAAA-DDDD, Cation, Leigh

N	3.445514	-0.457157	-0.242725
C	2.308709	0.335964	-0.208178
C	2.404745	1.771008	-0.285995
C	3.715661	2.384111	-0.469257
C	4.824461	1.519398	-0.537150
C	4.601624	0.107058	-0.399663
C	1.233340	2.484402	-0.167225
C	0.010058	1.807763	-0.026236
C	0.010931	0.378992	-0.033225
N	1.163546	-0.325301	-0.097589
C	6.113094	2.041259	-0.715741
C	6.297263	3.405648	-0.827148
C	5.204299	4.292550	-0.763851
C	3.927294	3.761750	-0.586532
N	-1.139380	-0.327615	0.023982
C	-2.286560	0.331199	0.140055
C	-2.384267	1.764727	0.234304
C	-1.212784	2.481289	0.122496
N	-3.421937	-0.462123	0.163740
C	-4.578576	0.100583	0.327203
C	-4.800377	1.510143	0.485155
C	-3.693904	2.373665	0.428808
C	-6.092073	2.031064	0.678100
C	-6.268375	3.388779	0.816423
C	-5.170925	4.279803	0.766226
C	-3.899619	3.755615	0.571963
C	5.374200	5.809595	-0.880603
C	4.563706	6.316533	-2.086243
C	-5.425373	5.777901	0.933683
C	-6.385266	6.252199	-0.171772
C	4.852802	6.473408	0.405850
C	6.838633	6.213721	-1.076322
C	-6.065511	6.023620	2.311460
C	-4.136306	6.600276	0.841745
H	5.469776	-0.552175	-0.422617
H	6.961574	1.365149	-0.764290
H	7.300552	3.789570	-0.963729
H	3.082281	4.440480	-0.543213
H	1.226521	3.569575	-0.179727
H	-1.207253	3.566219	0.146662
H	-3.050813	4.426176	0.537835
H	-7.269057	3.780090	0.967279
H	-6.940859	1.354914	0.717544
H	-5.446658	-0.558902	0.341433
H	6.903374	7.302419	-1.153680
H	7.256585	5.789234	-1.994301
H	7.460574	5.902444	-0.231470
H	3.496228	6.105756	-1.976659
H	4.911557	5.849870	-3.012704
H	4.683380	7.400156	-2.181466
H	3.794020	6.257206	0.574251
H	4.966324	7.559421	0.332817
H	5.415164	6.126725	1.277993
H	-3.649278	6.480995	-0.131342
H	-3.424203	6.326272	1.626658
H	-4.375848	7.659840	0.966257
H	-5.953381	6.080512	-1.162301
H	-6.572911	7.324460	-0.059454
H	-7.348636	5.737414	-0.123763
H	-5.403755	5.683553	3.113681
H	-7.022379	5.504234	2.413556
H	-6.248508	7.093998	2.446680
C	-5.841858	-3.829889	-1.196903
C	-4.480003	-4.029288	-0.975798
C	-3.887934	-5.306146	-1.040832
C	-4.663918	-6.430309	-1.331705
C	-6.020722	-6.238110	-1.548639
C	-6.599910	-4.957995	-1.482010
N	-2.527351	-5.207774	-0.784565
C	-2.333414	-3.927875	-0.574013
N	-3.444571	-3.160287	-0.676441
N	-1.111547	-3.331642	-0.276149
C	0.008955	-4.038391	0.001274
N	0.008916	-5.350055	0.022243
N	1.129804	-3.323567	0.255548
C	2.351497	-3.910526	0.572171
N	3.464729	-3.142252	0.640496

C	4.499204	-4.000830	0.971416
C	3.904589	-5.273078	1.087151
N	2.543514	-5.181848	0.830984
C	5.861980	-3.795881	1.181196
C	6.618413	-4.913714	1.508268
C	6.036703	-6.189148	1.626104
C	4.679088	-6.386802	1.419693
H	-3.484575	-2.157626	-0.416519
H	-1.088333	-2.301895	-0.189690
H	-4.211040	-7.414315	-1.385091
H	-6.650425	-7.091156	-1.777676
H	-7.664374	-4.848163	-1.660008
H	-6.289165	-2.843177	-1.152626
H	0.879835	-5.816138	0.290455
H	-0.862958	-5.824375	-0.227803
H	1.106671	-2.296642	0.140317
H	3.505256	-2.147682	0.351266
H	6.311558	-2.812844	1.096893
H	7.683528	-4.799299	1.679346
H	6.665145	-7.034107	1.886293
H	4.224398	-7.367073	1.512030

AAAA-DDDD, cation, 2CH-N, Leigh

C	4.962479	-1.518749	-0.488337
C	4.070409	-2.235332	0.279966
N	4.763587	-3.087025	1.068141
N	6.037265	-2.933341	0.829554
N	6.164485	-1.994141	-0.093725
N	2.678605	-2.128488	0.280000
C	1.821811	-3.082507	0.687684
N	2.251831	-4.219496	1.206365
C	7.489516	-1.537789	-0.528523
C	8.527115	-2.651557	-0.487850
C	9.882657	-2.150235	-0.982944
C	10.962857	-3.228764	-0.913683
C	12.319936	-2.724914	-1.396848
N	0.509980	-2.828496	0.526884
C	-0.527546	-3.720598	0.823228
C	-1.851001	-3.612221	0.458551
N	-2.403407	-4.718879	0.997767
N	-1.511643	-5.464667	1.630879
N	-0.358948	-4.858298	1.534273
C	-3.796102	-5.151696	0.897793
C	-3.937227	-6.406864	0.043745
C	-5.403178	-6.792020	-0.139564
C	-5.577130	-8.086126	-0.932317
C	-7.045759	-8.441648	-1.148146
N	2.671468	0.756531	-0.069035
C	3.616165	1.633044	0.051155
C	3.424987	3.057682	0.126194
C	2.117893	3.570095	0.068222
C	1.031330	2.604001	-0.044853
C	1.357938	1.203255	-0.105552
C	4.517854	3.933218	0.245968
C	4.306244	5.292224	0.304346
C	3.001077	5.833903	0.243914
C	1.927280	4.960995	0.126732
C	-0.306183	2.938825	-0.085958
C	-1.280603	1.930434	-0.181285
C	-0.852744	0.568435	-0.233515
N	0.456605	0.235721	-0.191193
N	-1.725673	-0.455259	-0.328339
C	-3.021063	-0.182037	-0.372649
C	-3.560797	1.155529	-0.305654
C	-2.662222	2.195768	-0.215731
C	-5.009903	1.328932	-0.333676
C	-5.791315	0.164014	-0.448167
C	-5.123881	-1.111949	-0.529215
N	-3.844755	-1.295227	-0.493842
C	-5.654660	2.568059	-0.246639
C	-7.044369	2.673607	-0.268791
C	-7.803494	1.493169	-0.386097
C	-7.188452	0.258471	-0.474592
C	2.823425	7.351458	0.309697
C	3.402247	7.867033	1.639577
C	-7.691220	4.057402	-0.164905
C	-7.254581	4.723507	1.151511
C	-7.230224	4.918661	-1.353719
C	-9.221362	3.983372	-0.183609
C	3.580376	7.996948	-0.864752
C	1.352038	7.768275	0.226389
H	4.836792	-0.768962	-1.252259
H	2.321197	-1.211157	-0.004071
H	1.564204	-4.892660	1.537245
H	3.243367	-4.318300	1.402307
H	0.246294	-1.928748	0.117309
H	-2.416367	-2.866782	-0.083588
H	-5.746594	-2.002828	-0.625917
H	-7.782247	-0.646990	-0.561700
H	-8.885277	1.541616	-0.405929
H	-5.064739	3.473977	-0.153662
H	-2.994016	3.228414	-0.169852
H	-0.632524	3.973402	-0.040825
H	0.922152	5.360143	0.078445
H	5.158574	5.957660	0.396944
H	5.524171	3.526859	0.291341
H	4.637988	1.253305	0.097316
H	-9.631737	4.993633	-0.101395
H	-9.607163	3.397480	0.656544
H	-9.595069	3.546720	-1.114944
H	-6.170238	4.856752	1.199799
H	-7.563525	4.123210	2.012618
H	-7.717654	5.711440	1.237373
H	-6.144376	5.048936	-1.362619
H	-7.687438	5.911149	-1.290888
H	-7.527369	4.462037	-2.302715
H	0.767798	7.356733	1.055963
H	0.895439	7.450051	-0.716114
H	1.282730	8.858441	0.279297
H	2.881639	7.417111	2.490996
H	3.281873	8.953359	1.697376
H	4.468231	7.642023	1.733009
H	3.192070	7.636888	-1.822076
H	4.651383	7.779871	-0.826244
H	3.456955	9.083984	-0.829452
H	-4.344105	-4.311526	0.462631
H	-4.167148	-5.319207	1.912213
H	-3.470767	-6.229805	-0.932604
H	-3.387471	-7.224372	0.523010
H	-5.879810	-6.903141	0.843474
H	-5.932086	-5.976814	-0.651744
H	-5.072897	-7.986367	-1.902440
H	-5.070897	-8.902017	-0.402332
H	-7.153747	-9.383601	-1.692650
H	-7.565451	-8.544978	-0.190263
H	-7.554874	-7.659900	-1.721314
H	7.366367	-1.155010	-1.545160
H	7.786916	-0.704484	0.116402
H	8.619115	-3.024129	0.536861
H	8.184614	-3.489260	-1.106191
H	9.790121	-1.791992	-2.017162
H	10.195495	-1.286297	-0.380635
H	11.046752	-3.585748	0.120214
H	10.651333	-4.091443	-1.515310
H	13.084360	-3.503154	-1.326165
H	12.265946	-2.398487	-2.440103
H	12.652213	-1.871428	-0.797081

AAAA-DDDD, cation, model

H	3.879317	-4.030777	-1.163620
C	4.118653	-2.991449	-0.918379
N	3.243676	-2.150441	-0.521212
C	1.944153	-2.635450	-0.399577
N	1.007788	-1.815609	-0.101629
C	-0.264470	-2.362978	0.026086
N	-1.259413	-1.580052	0.183405
C	-2.512069	-2.198799	0.335889
N	-3.529256	-1.477792	0.543037
C	-4.809273	-2.138876	0.714065
H	1.767229	-3.708280	-0.561265
H	-0.368537	-3.455998	-0.002289
H	-2.551260	-3.295825	0.273048
N	-3.162259	1.198612	-0.683756
H	-4.059952	1.634505	-0.835890
C	-2.103901	2.047887	-0.608080
N	-0.913429	1.385459	-0.239556
C	0.277340	1.993120	-0.007733
N	1.308994	1.174980	0.327147
C	2.613978	1.598756	0.650277
N	3.448613	0.545963	0.889822
H	4.419332	0.793401	1.017085
N	-2.076325	3.301618	-0.876305
N	0.423476	3.288284	-0.099123
N	2.873670	2.848966	0.747655
H	3.311294	-0.324103	0.376179
H	1.147343	0.164112	0.283676
H	-0.411493	3.807886	-0.401696
H	1.351570	3.653035	0.145851
H	-0.976159	0.370557	-0.090604
H	-3.194206	0.343898	-0.121386
H	5.150691	-2.665831	-1.022742
H	-3.001506	3.654804	-1.103087
H	3.853418	3.011766	0.962128
H	-5.542881	-1.662624	0.059594
H	-4.773791	-3.213143	0.499339
H	-5.145612	-1.990563	1.744003

AAAA-DDDD, neutral, Leigh

C	4.284497	3.202241	-0.766611
C	3.899593	1.850835	-0.761446
C	4.870606	0.865081	-1.001134
C	6.204167	1.235778	-1.243479
C	6.557979	2.566097	-1.241452
C	5.600472	3.578351	-0.999593
C	2.537137	1.395412	-0.510971
C	2.266153	-0.020373	-0.507333
N	3.274324	-0.946833	-0.734895
C	4.473367	-0.517900	-0.966197
C	1.475071	2.238514	-0.264658
C	0.194422	1.707397	-0.034930
C	0.027721	0.288452	-0.064319
N	1.067694	-0.542063	-0.291549
N	-1.180633	-0.286523	0.130232
C	-2.226184	0.491965	0.359810
C	-2.160622	1.930439	0.428789
C	-0.929753	2.512435	0.221862
C	-3.383990	2.679332	0.701191
C	-4.561514	1.933877	0.898288
C	-4.497058	0.499782	0.786728
N	-3.428502	-0.182856	0.531532
C	-5.771211	2.588715	1.162994
C	-5.814080	3.968502	1.225414
C	-4.651834	4.738275	1.024406
C	-3.452436	4.075547	0.768915
C	-4.664953	6.268673	1.069375
C	-6.060910	6.826243	1.365961
C	6.050797	5.039692	-0.998230
C	4.894822	6.004041	-0.715523
C	-3.704486	6.752190	2.169629
C	-4.202378	6.814629	-0.292862
C	7.122576	5.231093	0.089719
C	6.646997	5.383839	-2.374174
H	-5.422201	-0.064509	0.913078
H	-6.673251	2.002285	1.312941
H	-6.760740	4.454615	1.426955
H	-2.553812	4.663323	0.612512
H	-0.799758	3.589754	0.252702
H	1.600603	3.316374	-0.244858
H	3.539689	3.965448	-0.580999
H	7.591912	2.838976	-1.426598
H	6.947265	0.464839	-1.424877
H	5.240027	-1.274608	-1.136902
H	-6.014611	7.918614	1.390119
H	-6.434900	6.486389	2.336782
H	-6.782920	6.540309	0.594692

H	-2.676964	6.427598	1.983035
H	-4.011091	6.370956	3.148281
H	-3.709410	7.845966	2.209193
H	-3.187073	6.488955	-0.536504
H	-4.209961	7.908951	-0.274504
H	-4.869684	6.479178	-1.092456
H	4.448023	5.823183	0.267288
H	4.111098	5.928461	-1.475993
H	5.271036	7.030753	-0.726146
H	6.722101	4.981490	1.077023
H	7.450790	6.275064	0.104933
H	8.001115	4.605565	-0.090994
H	5.901660	5.250765	-3.164105
H	7.512061	4.758441	-2.611663
H	6.975144	6.427953	-2.383135
N	-3.770180	-2.788786	-0.699981
C	-2.768305	-3.715514	-0.765160
N	-3.141687	-4.878604	-1.251705
C	-4.493482	-4.716202	-1.520013
C	-4.907427	-3.409957	-1.180492
C	-5.416713	-5.622215	-2.044497
C	-6.729322	-5.195189	-2.214106
C	-7.124557	-3.892046	-1.872740
C	-6.217977	-2.973914	-1.350236
N	-1.513044	-3.365224	-0.336881
C	-0.461745	-4.272656	-0.148119
N	-0.474842	-5.527225	-0.334512
N	0.670261	-3.579531	0.288827
C	1.812565	-4.180938	0.774316
N	1.901879	-5.272044	1.495310
C	3.256069	-5.389770	1.762876
C	3.971526	-4.312761	1.191836
N	3.011416	-3.555000	0.554791
C	3.942651	-6.366539	2.489002
C	5.320404	-6.238407	2.622175
C	6.014670	-5.160378	2.048405
C	5.350838	-4.176321	1.322769
H	3.134805	-2.702455	-0.000151
H	0.767024	-2.602640	0.005707
H	3.404685	-7.197977	2.933460
H	5.873674	-6.985808	3.181502
H	7.090917	-5.093753	2.172164
H	5.884895	-3.342378	0.878940
H	-1.406749	-5.816249	-0.630019
H	-1.383146	-2.396404	-0.039961
H	-3.682946	-1.863389	-0.262507
H	-6.520299	-1.965324	-1.087935
H	-8.157452	-3.593131	-2.019043
H	-7.465032	-5.882286	-2.619377
H	-5.108293	-6.628555	-2.307877

AAAA-DDDD, neutral, model

C	-5.426139	1.285152	0.678116
N	-4.276971	0.744077	0.557619
C	-3.242415	1.609593	0.202006
N	-2.045896	1.159501	0.177542
C	-1.066994	2.063450	-0.221635
N	0.163205	1.739872	-0.128470
C	1.076648	2.706442	-0.578308
N	2.314846	2.530112	-0.392804
C	3.220199	3.557715	-0.869567
H	-5.603948	2.356192	0.531093
H	-3.494487	2.651079	-0.050567
H	-1.393191	3.036829	-0.616671
H	0.671094	3.594629	-1.086974
H	-6.276503	0.661771	0.943798
H	3.962794	3.098026	-1.526651
H	2.713793	4.368299	-1.407442
H	3.757557	3.977575	-0.014577
N	3.475098	0.254843	1.286438
C	3.083560	-0.981077	0.776507
N	3.759305	-2.066474	0.821087
N	1.788167	-0.906495	0.269553
C	1.007848	-1.944162	-0.250611
N	1.485891	-3.002015	-0.758501
N	-0.357709	-1.603221	-0.131831
C	-1.429104	-2.439086	-0.416585
N	-1.268969	-3.542800	-1.054869
N	-2.618363	-1.977359	0.110899
H	4.472522	0.321212	1.435526
H	-3.447551	-2.354059	-0.324863
H	-2.693673	-0.987374	0.313358
H	-0.582382	-0.749994	0.365595
H	0.704361	-3.596347	-1.041064
H	1.324689	-0.008839	0.370324
H	3.106986	1.063598	0.783919
H	4.666213	-1.862435	1.241518
H	-2.160116	-4.028609	-1.132492

ADA-DAD

H	-0.771790	-0.606447	0.109400
N	-0.027664	-1.325076	0.135852
C	1.205731	-0.890897	0.546069
N	2.195912	-1.851576	0.580359
C	1.941095	-3.140468	0.187202
C	0.725923	-3.558457	-0.223359
C	-0.367525	-2.611250	-0.260271
O	1.416645	0.275233	0.865843
C	3.549764	-1.422548	0.959482
H	2.795357	-3.806891	0.235603
H	0.544125	-4.581106	-0.520064
O	-1.519667	-2.862134	-0.604850
H	4.073619	-2.305272	1.334925
C	4.295041	-0.793035	-0.211843
H	3.446528	-0.709284	1.779476
C	5.695574	-0.333092	0.185837
H	4.358120	-1.520504	-1.031000
H	3.711656	0.060169	-0.577558
C	6.444964	0.324267	-0.971964
H	5.623742	0.376801	1.020929
H	6.274769	-1.190553	0.554866
C	7.847692	0.778799	-0.577629
H	6.505013	-0.382374	-1.809212
H	5.863471	1.182207	-1.331602
H	8.363862	1.254802	-1.415262
H	7.806719	1.499119	0.245679
H	8.454531	-0.070316	-0.247403
N	-2.193303	0.779603	0.009467
C	-1.886658	2.085828	0.036512
C	-2.852848	3.093370	-0.037595
C	-4.177428	2.693489	-0.138138
C	-4.523954	1.350417	-0.165912
C	-3.482313	0.419934	-0.091744
N	-0.520346	2.348231	0.168247
H	-2.559772	4.130463	-0.014556
H	-4.957780	3.445737	-0.197088
H	-5.545896	1.016657	-0.243896
N	-3.686374	-0.961596	-0.139280
H	-2.850203	-1.535200	-0.263386
C	-4.884236	-1.631421	-0.075391
C	0.115892	3.558808	0.040562
H	0.068229	1.545699	0.390446
O	-5.969090	-1.086227	0.053400
C	-4.765100	-3.136063	-0.179675
O	-0.450639	4.607568	-0.224233
C	1.612295	3.503608	0.256828
H	-3.734135	-3.486394	-0.215483
H	-5.280793	-3.578413	0.674767
H	-5.290100	-3.456105	-1.082796
H	1.988247	2.494668	0.423880
H	2.098373	3.942423	-0.616634
H	1.855063	4.129767	1.118362

ADDA-DAAD, Yosuke

N	-3.456081	-0.143760	0.642792
C	-2.340339	0.612900	0.556312
C	-2.686303	1.927547	0.797579
N	-4.021916	1.859624	1.022767
N	-4.475724	0.623034	0.925784
N	-1.128056	0.006812	0.273323
C	-0.016699	0.753860	-0.011730
O	-0.016439	1.980415	-0.016207
C	-4.944810	2.954524	1.305006
C	-5.067818	3.923528	0.132858
C	-6.132026	4.984322	0.404737
C	-6.219361	6.031509	-0.704238
C	-7.327573	7.055254	-0.468706
C	-7.372411	8.127951	-1.552844
N	1.094063	0.004199	-0.292481
C	2.305075	0.607962	-0.585621
N	3.420258	-0.149275	-0.675388
N	4.437521	0.615087	-0.973677
N	3.982589	1.850483	-1.077451
C	2.649145	1.920924	-0.839841
C	4.904697	2.946837	-1.355617
C	5.146623	3.817912	-0.127149
C	6.185453	4.900364	-0.410467
C	6.408838	5.828643	0.781534
C	7.477644	6.887499	0.520527
C	7.673810	7.825548	1.708721
N	3.439133	-2.974404	0.063495
C	4.749427	-3.362813	0.264027
O	5.096117	-4.493728	0.560482
C	2.293867	-3.756651	0.090455
N	1.145395	-3.092231	0.032058
C	-0.015374	-3.804876	0.015378
C	-0.014430	-5.222703	0.028615
C	1.225659	-5.892788	0.100601
C	2.385411	-5.178613	0.143916
N	-1.177016	-3.094325	-0.014500
C	-2.324717	-3.761103	-0.060995
C	-2.414345	-5.183985	-0.088011
C	-1.253691	-5.895652	-0.031377
N	-3.470867	-2.980014	-0.048694
C	-4.780653	-3.373332	-0.243208
O	-5.125698	-4.508903	-0.523097
C	5.740453	-2.227466	0.085287
C	7.182977	-2.686100	0.239815
C	8.179791	-1.545421	0.051923
C	9.628262	-2.013216	0.169359
C	10.648844	-0.893466	-0.018460
C	12.091506	-1.382043	0.088144
C	13.124550	-0.273822	-0.100769
C	14.563301	-0.774666	0.002784
C	15.603104	0.327127	-0.185365
C	17.040229	-0.179450	-0.083221
C	18.070841	0.930632	-0.271090
C	-5.773127	-2.236823	-0.079966
C	-7.214829	-2.696499	-0.238508
C	-8.212036	-1.554852	-0.058847
C	-9.660419	-2.020898	-0.184511
C	-10.680106	-0.899395	-0.002682
C	-12.123283	-1.384837	-0.116920
C	-13.154521	-0.274053	0.066466
C	-14.594089	-0.771457	-0.041202
C	-15.631468	0.333472	0.141925
C	-17.069770	-0.169505	0.038315
C	-18.097526	0.943989	0.221438
H	3.314155	-1.982452	-0.169973
H	1.081408	-1.018021	-0.198825
H	-1.114797	-1.016291	0.191648
H	-3.346902	-1.983862	0.167345
H	-1.268260	-6.981719	-0.028581
H	1.241618	-6.978860	0.117946
H	-5.612639	-1.773643	0.901234
H	-5.525246	-1.453842	-0.808117
H	5.574516	-1.772062	-0.898531
H	5.496570	-1.438770	0.808683
H	-7.345565	-3.153267	-1.225955
H	-7.422730	-3.486804	0.492210
H	-8.062278	-1.088578	0.924602
H	-8.013099	-0.771702	-0.803220
H	-9.806451	-2.487976	-1.168079
H	-9.850887	-2.806770	0.559203
H	-10.531656	-0.427894	0.978527

H	-10.498870	-0.115950	-0.751332
H	-12.270118	-1.857604	-1.097698
H	-12.300053	-2.170012	0.631149
H	-13.006633	0.201228	1.045955
H	-12.983312	0.509406	-0.684450
H	-14.740875	-1.247980	-1.020265
H	-14.763008	-1.555413	0.709826
H	-15.484614	0.812261	1.120008
H	-15.466475	1.116760	-0.610876
H	-17.213344	-0.649129	-0.937989
H	-17.232074	-0.950630	0.791692
H	-19.120162	0.565237	0.146332
H	-17.985545	1.418902	1.201406
H	-17.969577	1.720358	-0.539529
H	7.317694	-3.139349	1.228277
H	7.387934	-3.479056	-0.488909
H	8.024451	-1.080452	-0.931295
H	7.986267	-0.761090	0.796412
H	9.779162	-2.480284	1.152018
H	9.813419	-2.799605	-0.575170
H	10.496012	-0.422152	-0.998999
H	10.473067	-0.109551	0.730850
H	12.242222	-1.854732	1.068307
H	12.262802	-2.167882	-0.660384
H	12.974314	0.200450	-1.080371
H	12.957928	0.511076	0.649768
H	14.711931	-1.250127	0.981897
H	14.727636	-1.560235	-0.747624
H	15.455599	0.803961	-1.164331
H	15.441685	1.112645	0.565824
H	17.184234	-0.656974	0.894078
H	17.199039	-0.963027	-0.834779
H	19.092563	0.549313	-0.196365
H	17.958805	1.403031	-1.252246
H	17.946009	1.709548	0.487789
H	-5.902748	2.477285	1.523547
H	-4.599603	3.469704	2.206501
H	5.830385	2.475050	-1.692728
H	4.493213	3.534054	-2.181682
H	-4.099096	4.404967	-0.048465
H	-5.322998	3.358036	-0.771088
H	-7.107963	4.494270	0.523411
H	-5.917341	5.484419	1.359261
H	-5.254512	6.551395	-0.788372
H	-6.386214	5.531687	-1.668645
H	-8.292557	6.536186	-0.421380
H	-7.181906	7.525243	0.511611
H	-8.175430	8.847656	-1.373157
H	-6.427677	8.679931	-1.592046
H	-7.536134	7.679445	-2.538062
H	4.201320	4.278709	0.184940
H	5.482814	3.179376	0.698560
H	7.136698	4.426159	-0.687454
H	5.869724	5.494298	-1.279184
H	5.461855	6.322680	1.038962
H	6.695174	5.232887	1.659089
H	8.425755	6.390063	0.280796
H	7.199919	7.468152	-0.368232
H	8.442889	8.575687	1.507392
H	6.743936	8.352427	1.945299
H	7.974950	7.266831	2.600749
H	3.354568	-5.647133	0.204020
H	-3.382718	-5.654772	-0.140058
H	2.080084	2.832567	-0.865022
H	-2.115876	2.838510	0.820468

ADDA-DAAD, yosuke, model

C	0.157842	-2.889723	-1.770070
C	0.009538	-1.912809	-0.863781
N	1.084422	-1.341394	-0.156527
C	1.908991	-2.119387	0.427842
N	3.036934	-1.614191	1.025043
N	-1.193291	-1.226280	-0.601652
C	-2.270433	-1.911959	-0.594432
N	-3.486380	-1.304566	-0.414041
N	-3.160586	1.416835	0.801077
C	-2.132964	2.411755	0.622749
N	-0.966601	1.784761	0.185089
C	0.209927	2.453706	-0.082351
O	0.312747	3.671291	-0.064121
N	1.256201	1.604566	-0.361438
C	2.541708	2.030483	-0.688815
N	3.461382	0.935804	-0.507834
H	1.789359	-3.202363	0.500473
H	-2.316302	-2.995356	-0.720431
C	-4.664471	-2.016557	-0.406060
C	3.904510	-2.404610	1.743835
C	-2.389512	3.710373	0.810397
N	-3.972854	1.670927	1.699514
N	4.419127	0.929418	-1.292259
H	-3.476845	-0.297817	-0.228914
H	-1.023169	0.774761	0.024760
H	1.138695	0.589710	-0.250472
H	3.245340	-0.629296	0.846964
C	2.972209	3.249153	-1.029810
H	1.134359	-3.314507	-1.966273
H	-0.677672	-3.229729	-2.369364
O	-4.734920	-3.213954	-0.574420
H	-5.542978	-1.376749	-0.234386
O	3.731896	-3.585592	1.949652
H	4.776150	-1.844450	2.113262
H	-4.670684	0.910879	1.695958
H	5.012715	0.129714	-1.022857
H	-1.646200	4.467854	0.625303
H	-3.381865	3.981358	1.145642
H	4.031821	3.381337	-1.204904
H	2.296935	4.086971	-1.099474

Coordinates of Base Pairs

AA1

N	0.138260	1.941355	0.000106
C	0.806830	0.771262	0.000103
C	0.250573	-0.517053	-0.000278
C	-1.164922	-0.600050	-0.000398
N	-1.859417	0.571439	-0.000494
C	-1.186007	1.738560	-0.000272
N	1.234723	-1.490862	-0.000435
C	2.363615	-0.802405	-0.000094
N	2.167963	0.561347	0.000290
N	-1.831615	-1.763199	-0.000499
H	-1.811096	2.636502	-0.000406
H	-2.876145	-1.788372	-0.000243
H	-1.296130	-2.625585	0.000429
H	3.363010	-1.231058	-0.000174
H	2.889011	1.278652	0.000701
N	-4.740101	-1.784098	-0.000213
C	-5.426902	-0.607409	-0.000834
C	-6.843081	-0.679600	-0.001322
C	-7.409057	-1.963516	-0.001521
N	-6.749387	-3.138605	-0.001073
C	-5.423495	-2.945812	-0.000352
N	-4.753380	0.551539	-0.000991
N	-7.819832	0.301577	-0.002013
N	-8.768593	-1.743392	-0.002329
H	-4.806559	-3.849499	0.000217
H	-5.283921	1.417255	-0.001268
H	-3.708002	0.570566	-0.000815
H	-9.494060	-2.456205	-0.002977
C	-8.954078	-0.378128	-0.002589
H	-9.949537	0.059628	-0.003287

AA2

C	-9.055601	-0.686466	-0.002349
N	-7.951229	0.042731	-0.002129
C	-6.919242	-0.884287	-0.001579
C	-7.432418	-2.192079	-0.001420
N	-8.802696	-2.034622	-0.001981
N	-6.731873	-3.338947	-0.000980
C	-5.410349	-3.092765	-0.000693
N	-4.772239	-1.910581	-0.000846
C	-5.503998	-0.763208	-0.001341
N	-4.858261	0.413759	-0.001676
N	-5.785265	3.163099	-0.002195
C	-7.020926	3.732934	-0.002300
C	-7.086886	5.149173	-0.002430
C	-5.863559	5.836873	-0.002701
N	-4.630607	5.293832	-0.002651
C	-4.695578	3.955962	-0.002351
N	-8.157856	6.026409	-0.002448
C	-7.590864	7.221218	-0.002794
N	-6.214100	7.168461	-0.002963
N	-8.108705	2.949299	-0.002223
H	-3.736098	3.429275	-0.002273
H	-8.022532	1.912266	-0.002167
H	-9.023153	3.389673	-0.003506
H	-8.121506	8.170460	-0.002790
H	-5.574844	7.959492	-0.003352
H	-4.762060	-3.974266	-0.000283
H	-5.338997	1.337473	-0.001898
H	-3.842470	0.384848	-0.000891
H	-9.492474	-2.781993	-0.002009
H	-10.069341	-0.293823	-0.003010

AA3

N	0.035508	2.163336	-0.000172
C	0.785584	1.048272	-0.000027
C	0.328152	-0.279945	0.000097
C	-1.079338	-0.459901	0.000071
N	-1.861389	0.652077	-0.000047
C	-1.273961	1.861039	-0.000158
N	1.395050	-1.165141	0.000228
C	2.467649	-0.389909	0.000188
N	2.160927	0.947483	0.000015
N	-1.668241	-1.667145	0.000244
H	-1.959348	2.713719	-0.000256
H	-2.683731	-1.693532	-0.000227
H	-1.138796	-2.556899	0.000092
H	3.497148	-0.739698	0.000272
H	2.820160	1.721986	0.000050
H	1.825560	-3.036014	0.000136
N	2.353968	-3.926527	0.000050
H	3.369459	-3.901473	-0.000449
C	1.765088	-5.133804	-0.000197
N	2.547369	-6.245750	-0.000337
C	1.960432	-7.455042	-0.000446
N	0.651091	-7.757559	-0.000421
C	-0.099076	-6.642460	-0.000305
C	0.357883	-5.314018	-0.000236
H	2.646128	-8.307789	-0.000521
N	-1.474390	-6.541925	-0.000267
N	-0.709049	-4.429044	-0.000160
C	-1.781386	-5.204663	-0.000156
H	-2.133704	-7.316389	-0.000088
H	-2.810914	-4.855044	-0.000118

AC1

N	0.082723	1.936678	0.000155
C	0.775228	0.780325	0.000179
C	0.246989	-0.519573	0.000084
C	-1.167518	-0.634490	-0.000033
N	-1.886584	0.525228	-0.000167
C	-1.236666	1.705047	-0.000047
N	1.252638	-1.471163	-0.000038
C	2.366412	-0.758476	-0.000004
N	2.140500	0.600777	0.000181
N	-1.811359	-1.807430	-0.000085
H	-1.879570	2.590457	-0.000123
H	-2.857171	-1.845760	-0.000259
H	-1.266802	-2.664297	0.000551
H	3.374985	-1.164936	-0.000170

H	2.844159	1.335039	0.000126
N	-4.688789	-1.795211	-0.000863
C	-5.431436	-0.673432	-0.001316
C	-6.870365	-0.711069	-0.001583
C	-7.456586	-1.941533	-0.001544
N	-6.689994	-3.065428	-0.001227
C	-5.273405	-3.028808	-0.000653
N	-4.781627	0.501603	-0.001531
H	-7.465152	0.200020	-0.001855
H	-8.536493	-2.089497	-0.001777
H	-7.121474	-3.987373	-0.001022
O	-4.641761	-4.094396	-0.000048
H	-5.311298	1.366529	-0.001819
H	-3.734077	0.527243	-0.001150

AC2

N	0.041909	2.109639	-0.000264
C	0.776292	0.983637	-0.000165
C	0.302610	-0.338260	-0.000094
C	-1.110059	-0.504214	-0.000019
N	-1.875206	0.622773	-0.000077
C	-1.272045	1.822408	-0.000215
N	1.362556	-1.233938	-0.000008
C	2.444784	-0.472128	-0.000012
N	2.151389	0.867616	-0.000133
N	-1.712307	-1.700296	0.000148
H	-1.946356	2.684309	-0.000287
H	-2.728232	-1.729634	0.000400
H	-1.199146	-2.605118	0.000376
H	3.469704	-0.834548	-0.000122
H	2.818381	1.635309	0.000064
N	-0.649443	-4.392940	0.000576
C	0.573412	-4.950970	0.000421
C	0.764793	-6.377771	0.000033
C	-0.357060	-7.152040	0.000107
N	-1.587522	-6.571832	0.000423
C	-1.774884	-5.167378	0.000418
N	1.634055	-4.126802	0.000717
H	1.759087	-6.820160	-0.000202
H	-0.333331	-8.241907	-0.000051
H	-2.429771	-7.143137	0.000336
O	-2.927576	-4.712220	0.000327
H	2.570640	-4.515373	0.000091
H	1.502103	-3.092327	0.000568

AT (H)

N	0.172672	1.948752	0.000124
C	0.770057	0.744909	0.000010
C	0.137043	-0.507473	0.000026
C	-1.281027	-0.504906	0.000114
N	-1.909314	0.700012	0.000284
C	-1.165850	1.820548	0.000282
N	1.077384	-1.522753	-0.000120
C	2.249044	-0.907023	-0.000206
N	2.121045	0.457842	-0.000197
N	-2.017258	-1.629011	0.000067
H	-1.733049	2.756120	0.000410
H	-3.028874	-1.538847	-0.000231
H	-1.596467	-2.569693	0.000009
H	3.211103	-1.414165	-0.000379
H	2.879109	1.135847	-0.000038
H	1.025326	-3.243661	-0.000312
N	1.087233	-4.306191	-0.000352
C	2.365231	-4.825463	-0.000198
N	2.398090	-6.215462	-0.000143
C	1.269654	-6.997876	-0.000231
C	0.012054	-6.472803	-0.000371
C	-0.110649	-5.018204	-0.000400
O	3.386522	-4.133167	-0.000101
H	3.320348	-6.645114	-0.000105
H	1.454079	-8.072856	-0.000159
C	-1.225707	-7.326537	-0.000411
O	-1.195129	-4.402743	-0.000462
H	-2.115012	-6.682508	-0.000952
H	-1.268938	-7.973209	-0.890453
H	-1.269514	-7.972465	0.890146

AT (RH)

N	0.151448	1.908437	-0.000276
C	0.749493	0.705021	-0.000150
C	0.116884	-0.547690	0.000187
C	-1.300787	-0.545112	0.000231
N	-1.929861	0.658890	0.000141
C	-1.186865	1.779998	-0.000072
N	1.057570	-1.562371	0.000221
C	2.229074	-0.946469	-0.000096
N	2.100468	0.418404	-0.000383
N	-2.037905	-1.669586	0.000393
H	-1.753999	2.715612	-0.000090
H	-3.049485	-1.580272	0.000009
H	-1.618956	-2.608776	0.000264
H	3.190411	-1.455122	-0.000264
H	2.858147	1.096882	-0.000422
H	1.027419	-3.282403	0.000338
N	1.088387	-4.344853	0.000191
C	2.376485	-4.898919	0.000128
C	2.429482	-6.360021	-0.000314
C	1.252108	-7.041877	-0.000700
N	0.031942	-6.404028	-0.000628
C	-0.103327	-5.025480	-0.000184
O	3.368682	-4.156642	0.000420
C	3.767400	-7.032238	-0.000311
H	1.205488	-8.131197	-0.001069
H	-0.829885	-6.944405	-0.000844
O	-1.214419	-4.472017	-0.000172
H	3.656872	-8.125586	-0.000327
H	4.353727	-6.733548	-0.883930
H	4.353704	-6.733533	0.883312

AT (RWC)

N	-0.141568	1.887058	0.000350
C	0.633884	0.785364	0.000329
C	0.205764	-0.552537	-0.000014
C	-1.194153	-0.767911	-0.000364
N	-1.991435	0.333187	-0.000391
C	-1.440582	1.564356	-0.000050
N	1.279842	-1.425346	-0.000114
C	2.336025	-0.629967	0.000170
N	2.008299	0.708041	0.000486
N	-1.757967	-1.985846	-0.000874
H	-2.162083	2.387136	-0.000134
H	-2.784472	-2.085792	-0.000360
H	-1.163073	-2.807527	0.000424
H	3.372254	-0.959561	0.000399
H	2.654537	1.493417	0.000471
H	-3.710203	0.249685	-0.000414
N	-4.779300	0.199397	-0.000313
C	-5.328602	-1.057195	0.000005
N	-6.712953	-1.072426	0.000268
C	-7.478266	0.071326	0.000395
C	-6.931037	1.317396	0.000137
C	-5.469602	1.421830	-0.000296
O	-4.661308	-2.105635	0.000128
H	-7.156876	-1.987763	0.000557
H	-8.555694	-0.097491	0.000749
C	-7.761344	2.570922	0.000351
O	-4.831789	2.483424	-0.000615
H	-7.099218	3.446941	-0.000554
H	-8.407390	2.626970	-0.889499
H	-8.405867	2.627673	0.891266

AT (WC)

C	0.151985	1.935561	0.000130
N	0.710425	0.672246	0.000542
C	0.026535	-0.540826	0.000454
C	-1.428944	-0.458181	-0.000034
C	-1.992833	0.781336	-0.000400
N	-1.239447	1.929759	-0.000278
O	0.657107	-1.617810	0.000755
H	-1.692664	2.840590	-0.000530
O	0.813033	2.976077	0.000079
N	3.531858	-1.728611	-0.000200
C	4.199114	-0.565209	0.000134
C	5.612399	-0.469616	0.000324
C	6.153005	0.826750	0.000408
N	5.474470	1.990932	0.000392
C	4.152543	1.779956	0.000312
N	3.498542	0.600799	0.000179
N	6.608213	-1.431024	0.000167
C	7.728434	-0.728722	0.000172
N	7.516008	0.632589	0.000386
H	3.505268	2.662084	0.000371
H	2.497763	-1.737159	-0.000052
H	4.053711	-2.598648	0.000311
H	8.732824	-1.145445	0.000075
H	8.226939	1.360093	0.000405
H	1.781032	0.636890	0.000528
C	-2.227355	-1.725341	-0.000179
H	-3.072852	0.932369	-0.000820
H	-3.304800	-1.508494	-0.000348
H	-1.987611	-2.337491	-0.883932
H	-1.987863	-2.337550	0.883597

CC

C	-1.035454	1.253460	-0.000213
C	0.225384	1.770504	-0.000122
N	1.305994	0.942589	0.000137
C	1.190254	-0.469155	0.000062
N	-0.072032	-0.985031	0.000109
C	-1.154643	-0.182259	0.000053
O	2.220383	-1.159585	-0.000019
N	-2.360200	-0.767674	0.000268
H	2.250137	1.322291	0.000022
H	-2.440055	-1.813921	0.000420
H	-3.199470	-0.197972	-0.000101
H	-1.912248	1.897715	-0.000380
H	0.434029	2.840574	-0.000213
N	-2.471084	-3.638776	0.000894
C	-1.388289	-4.441340	0.001173
C	-1.506843	-5.876768	0.001258
C	-2.767296	-6.394490	0.001267
N	-3.848417	-5.567140	0.001138
C	-3.733280	-4.155221	0.000741
N	-0.182607	-3.856364	0.001435
H	-0.629287	-6.519928	0.001401
H	-2.974879	-7.464618	0.001402
H	-4.792350	-5.947314	0.000999
O	-4.763662	-3.465395	0.000314
H	0.656337	-4.426490	0.001103
H	-0.102659	-2.810289	0.000988

GA1

N	-0.681627	-1.419846	-0.163641
C	0.547046	-0.877436	-0.005349
C	0.898650	0.477589	0.116851
C	-0.149179	1.451761	0.097032
N	-1.415510	0.846493	-0.036099
C	-1.639516	-0.501018	-0.169369
N	2.269769	0.625454	0.240268
C	2.735944	-0.606851	0.195783
N	1.739923	-1.554222	0.047412
O	-0.054795	2.693070	0.180882
N	-2.949617	-0.889760	-0.262973
H	-2.258277	1.488228	0.030657
H	-3.610920	-0.219370	-0.645940
H	-3.093278	-1.851358	-0.559827
H	3.782897	-0.891723	0.264601
H	1.860008	-2.562360	-0.013644
N	-3.705406	2.519706	0.163073
C	-3.541420	3.852233	-0.076762
C	-4.706575	4.659342	-0.071745
C	-5.923334	4.011847	0.193500
N	-6.103612	2.699897	0.445248
C	-4.941647	2.038967	0.410469

N	-2.313176	4.334645	-0.311048
N	-4.890674	6.016925	-0.264189
N	-6.865767	5.013629	0.154114
H	-4.993900	0.965957	0.621162
H	-2.202641	5.338148	-0.420888
H	-1.473111	3.743564	-0.156572
H	-7.865526	4.906805	0.308254
C	-6.194533	6.184902	-0.121481
H	-6.720246	7.133119	-0.204735

GA2

H	-2.754191	-2.094546	0.003573
N	-2.647178	-1.056534	0.007297
H	-3.474872	-0.471430	0.001818
C	-1.422282	-0.500133	0.003756
N	-1.339782	0.877409	-0.001290
H	-2.202869	1.421279	-0.004661
C	-0.149676	1.666393	-0.003763
O	-0.231109	2.897737	-0.008192
C	1.007083	0.819294	-0.000796
N	2.353369	1.142377	-0.002590
C	2.970458	-0.020767	0.000915
H	4.047253	-0.170930	0.000759
N	2.093207	-1.092151	0.004871
H	2.346961	-2.076389	0.009041
C	0.821968	-0.572107	0.003809
N	-0.335316	-1.275459	0.006368
H	-0.267387	-3.207455	-0.002091
N	0.005018	-4.206445	-0.006979
H	0.989464	-4.458154	-0.005956
C	-0.880875	-5.218297	-0.005039
C	-2.286830	-5.029616	-0.003149
N	-3.092437	-3.901540	-0.002302
C	-4.329187	-4.373505	-0.000834
H	-5.233339	-3.770063	0.000046
N	-4.374518	-5.743881	-0.000759
H	-5.210356	-6.323554	0.000447
C	-3.071231	-6.195215	-0.002196
N	-2.634454	-7.465454	-0.002668
C	-1.291407	-7.511195	-0.004391
H	-0.848153	-8.511459	-0.004837
N	-0.413121	-6.493719	-0.005613

GA3

N	-0.607759	-1.505726	-0.284245
C	0.579623	-0.910322	-0.025347
C	0.849678	0.451753	0.191055
C	-0.247409	1.371055	0.164479
N	-1.467686	0.708038	-0.076583
C	-1.611620	-0.638927	-0.293994
N	2.201757	0.662118	0.400869
C	2.736177	-0.540229	0.315626
N	1.802723	-1.526972	0.058748
O	-0.230466	2.607103	0.322715
N	-2.895503	-1.085899	-0.481219
H	-2.344598	1.291834	-0.001093
H	-3.556296	-0.426937	-0.886243
H	-2.965904	-2.033432	-0.843721
H	3.791757	-0.774520	0.429184
H	1.980913	-2.522397	-0.050032
H	-1.557238	3.773925	-0.143824
N	-2.143540	4.590462	-0.388033
C	-3.476702	4.602818	-0.223076
H	-1.682949	5.489191	-0.505412
N	-4.140382	5.784639	-0.329659
C	-5.470754	5.806730	-0.147199
N	-6.299830	4.790280	0.148961
C	-5.625206	3.632424	0.233378
C	-4.246590	3.439619	0.046902
H	-5.940441	6.789870	-0.247106
N	-6.124660	2.377187	0.516541
N	-3.921703	2.100522	0.205465
C	-5.070472	1.503835	0.487843
H	-7.096481	2.148328	0.711360
H	-5.194674	0.442512	0.689654

GA4

N	-0.600969	-1.378428	0.003701
C	0.599787	-0.754064	0.001896
C	0.875674	0.622213	-0.000928
C	-0.223330	1.543341	-0.002355
N	-1.463318	0.834318	-0.001014
C	-1.637145	-0.534803	0.002510
N	2.240896	0.854846	-0.002111
C	2.779096	-0.347161	-0.000106
N	1.832671	-1.357890	0.002449
O	-0.223978	2.777386	-0.004531
N	-2.894078	-1.013128	0.006222
H	-2.289101	1.433308	-0.001750
H	-3.682561	-0.376114	-0.000212
H	-3.064816	-2.047871	0.003423
H	3.843533	-0.568302	-0.000510
H	2.016131	-2.357997	0.004564
N	-3.373746	-3.845466	-0.001066
C	-2.339438	-4.729941	-0.002180
C	-2.661185	-6.109951	-0.002100
C	-4.026000	-6.438323	-0.000980
N	-5.064129	-5.579634	0.000073
C	-4.639685	-4.309928	0.000009
N	-1.078368	-4.271190	-0.003463
N	-1.869666	-7.244818	-0.002671
N	-4.050981	-7.814700	-0.000971
H	-5.418467	-3.541474	0.000973
H	-0.319221	-4.944801	-0.003514
H	-0.881093	-3.250718	-0.001387
H	-4.881264	-8.402283	-0.000064
C	-2.740565	-8.239994	-0.001970
H	-2.488438	-9.297754	-0.002068

GC

N	-0.626935	-1.483366	-0.000097
C	0.589681	-0.902630	0.000165
C	0.913226	0.465875	-0.000324
C	-0.159330	1.408517	-0.002869
N	-1.414683	0.774278	-0.003713
C	-1.621142	-0.591068	-0.002179
N	2.286770	0.653637	-0.000133
C	2.782404	-0.567197	0.000479
N	1.804014	-1.545878	0.000734
O	-0.084591	2.657902	-0.004665
N	-2.902139	-1.010545	-0.005276
H	-2.255146	1.411270	-0.005925
H	-3.704560	-0.356282	0.004983
H	-3.065446	-2.011135	0.004617
H	3.839295	-0.822927	0.000610
H	1.947730	-2.552417	0.000469
N	-3.692444	2.536406	-0.008399
C	-3.539678	3.878428	-0.020257
C	-4.670021	4.768688	-0.020639
C	-5.907932	4.201669	-0.007354
N	-6.039042	2.845851	0.004160
C	-4.931558	1.978945	0.004418
N	-2.292586	4.362170	-0.031519
H	-4.542024	5.849186	-0.029773
H	-6.832434	4.778130	-0.004724
H	-6.960456	2.413244	0.016477
O	-5.137887	0.747493	0.016524
H	-1.470128	3.718676	-0.024024
H	-2.141559	5.365246	-0.040225

GC1

N	-0.553705	-1.482799	-0.001226
C	0.654079	-0.876374	-0.000237
C	0.952318	0.495264	-0.000172
C	-0.135007	1.433822	-0.000820
N	-1.385710	0.756037	-0.001884
C	-1.562200	-0.609387	-0.002479
N	2.322315	0.705770	0.000644
C	2.840996	-0.506184	0.001083
N	1.879174	-1.500653	0.000617
O	-0.097621	2.670233	-0.000506
N	-2.836601	-1.065399	-0.006201
H	-2.230662	1.364698	-0.001293
H	-3.661620	-0.441739	-0.000642
H	-2.961606	-2.071521	0.000411
H	3.902175	-0.743046	0.001626
H	2.038805	-2.504772	0.000686
O	-3.722388	2.380787	0.002499
C	-4.898467	1.976271	0.001894
N	-5.938793	2.925181	0.000347
C	-7.252055	2.575157	-0.001373
C	-7.609085	1.258671	-0.001383
C	-6.541033	0.300349	0.000832
N	-5.247571	0.657550	0.002641
H	-7.973153	3.392101	-0.002665
H	-8.653345	0.953970	-0.002794
N	-6.826164	-1.016901	0.001333
H	-5.661617	3.905288	-0.000070
H	-6.075543	-1.699824	0.002844
H	-7.784148	-1.347388	-0.001093

GC2

N	-0.608648	-1.381703	0.001278
C	0.598986	-0.771672	0.000581
C	0.892366	0.601040	-0.000264
C	-0.195292	1.535735	-0.000916
N	-1.443533	0.842657	-0.000579
C	-1.636625	-0.524765	0.000920
N	2.260612	0.816863	-0.000666
C	2.784183	-0.391333	-0.000197
N	1.825006	-1.390500	0.000571
O	-0.178911	2.769752	-0.001780
N	-2.896919	-0.987132	0.002845
H	-2.262445	1.451011	-0.000787
H	-3.681019	-0.344439	-0.001023
H	-3.080981	-2.020595	0.001717
H	3.845638	-0.626113	-0.000282
H	1.996468	-2.392568	0.000768
N	-3.357476	-3.805516	0.000534
C	-2.371869	-4.719917	0.000635
C	-2.640220	-6.133109	0.000255
C	-3.949834	-6.513036	0.000216
N	-4.934532	-5.574923	0.000425
C	-4.671171	-4.182915	0.000245
N	-1.105386	-4.269436	0.001081
H	-1.836689	-6.866808	0.000076
H	-4.270685	-7.554771	0.000044
H	-5.913926	-5.852062	0.000210
O	-5.619224	-3.386857	-0.000102
H	-0.338931	-4.933167	0.001098
H	-0.908038	-3.246694	0.001224

GG1

C	-1.064611	-1.468519	0.008267
C	0.258681	-0.938059	0.020257
N	0.256721	0.464322	0.025757
C	-0.862764	1.263029	0.018821
N	-2.105967	0.790907	-0.000457
C	-2.139396	-0.558682	-0.001817
O	1.349543	-1.559877	0.022542
N	-0.639888	2.601932	0.074378
N	4.587906	-2.252055	-0.098386
C	4.809105	-0.913226	-0.033407
N	6.051549	-0.439139	-0.020130
C	6.083354	0.910414	-0.013408
C	5.007791	1.819265	-0.014031
C	3.685303	1.286841	-0.015923
N	3.688695	-0.115711	-0.025675
N	5.461618	3.127807	-0.006968
C	6.774497	3.016158	-0.002295
N	7.204589	1.701572	-0.004632
O	2.593816	1.907455	-0.006820
H	2.753975	-0.602564	-0.021232
H	3.656687	-2.618045	0.082413
H	5.377777	-2.864334	0.076618

H	7.480831	3.842626	0.002243
H	8.167632	1.374270	-0.004322
H	1.191906	0.950684	0.029899
N	-3.261172	-1.349326	-0.016615
N	-1.519296	-2.776624	-0.000012
H	0.293082	2.963828	-0.105094
H	-1.427078	3.213562	-0.114191
C	-2.831957	-2.664322	-0.014067
H	-4.224049	-1.021737	-0.026769
H	-3.538009	-3.491175	-0.021789

GG3

N	-0.633536	-1.464628	0.001445
C	0.585614	-0.882576	0.001573
C	0.915284	0.483938	0.000625
C	-0.154806	1.439698	-0.002861
N	-1.413140	0.789860	-0.003234
C	-1.623092	-0.567900	-0.001471
N	2.289970	0.663548	0.000136
C	2.780877	-0.559952	0.000837
N	1.797316	-1.532492	0.001812
O	-0.099873	2.680744	-0.006056
N	-2.908103	-0.993499	-0.004994
H	-2.241343	1.440338	-0.008434
H	-3.719925	-0.365070	0.000733
H	-3.067642	-1.994474	0.003218
H	3.836488	-0.820739	0.000523
H	1.934524	-2.539909	0.001699
O	-5.539969	0.349344	0.009011
C	-5.783736	1.567073	0.002449
N	-7.123821	2.028984	0.010418
C	-7.523478	3.351347	0.005751
N	-6.673509	4.369340	-0.013214
C	-5.381526	3.973505	-0.014633
C	-4.875979	2.666434	-0.010899
H	-7.831993	1.294760	0.041809
N	-8.861892	3.588740	0.074225
N	-4.266727	4.778104	-0.028739
N	-3.497522	2.678522	-0.021043
H	-9.152952	4.546063	-0.101962
H	-9.515755	2.864306	-0.206435
C	-3.161775	3.954252	-0.031160
H	-4.261687	5.795492	-0.033376
H	-2.137899	4.320908	-0.039256

GG4

C	-6.949052	-4.557544	-0.004607
N	-6.477308	-5.786830	0.014230
C	-5.101972	-5.629308	0.011252
C	-4.751293	-4.271132	-0.010875
N	-5.948506	-3.600291	-0.020051
N	-3.516168	-3.715452	-0.021140
C	-2.530116	-4.614855	-0.009570
N	-2.777154	-5.970427	0.016050
C	-4.055878	-6.610179	0.026578
N	-1.246660	-4.205384	-0.038073
O	-4.122965	-7.841283	0.045750
N	-0.647217	-1.352129	0.027454
C	0.584142	-0.785780	0.015216
C	0.923639	0.575374	0.000956
C	-0.129922	1.548734	-0.003044
N	-1.403319	0.899226	0.007002
C	-1.639891	-0.458559	0.023588
N	2.297293	0.744658	-0.009136
C	2.779457	-0.480624	-0.001706
N	1.787290	-1.446465	0.013344
O	-0.071841	2.780334	-0.013683
N	-2.920302	-0.875622	0.046942
H	-2.199287	1.537463	0.006265
H	-3.675861	-0.202247	-0.006013
H	-3.136991	-1.894425	0.014720
H	3.832624	-0.750611	-0.006369
H	1.926249	-2.453683	0.019989
H	-1.986242	-6.614896	0.019324
H	-1.026169	-3.188215	-0.006680
H	-0.495630	-4.881542	0.042044
H	-6.077552	-2.591802	-0.036654
H	-7.999983	-4.279356	-0.008327

GT1

N	-0.697023	-1.372609	0.026708
C	0.535456	-0.816897	0.011528
C	0.889999	0.544712	0.001377
C	-0.162348	1.511566	0.003987
N	-1.426496	0.895561	0.026150
C	-1.660399	-0.457553	0.040657
N	2.265836	0.699967	-0.014647
C	2.733059	-0.532316	-0.014181
N	1.732877	-1.487463	0.000318
O	-0.080699	2.758684	-0.011401
N	-2.965486	-0.841391	0.120238
H	-2.252595	1.543111	0.028140
H	-3.691491	-0.168714	-0.111469
H	-3.165063	-1.817368	-0.074853
H	3.783754	-0.811897	-0.023754
H	1.852901	-2.497362	0.004760
O	-3.670242	2.485615	-0.006074
C	-3.604679	3.736558	-0.004407
C	-4.778798	4.592908	-0.002852
C	-4.578220	5.940575	-0.001011
N	-3.323859	6.492458	-0.000312
C	-2.148219	5.745797	-0.000826
N	-2.368550	4.374937	-0.002936
C	-6.138198	3.964406	-0.001535
H	-5.403122	6.653624	0.000493
H	-3.207979	7.503447	0.001040
O	-1.034275	6.261802	0.000210
H	-1.503248	3.773196	-0.005407
H	-6.922809	4.734066	-0.001457
H	-6.272577	3.320653	-0.884946
H	-6.271223	3.322191	0.883243

GT2

N	-2.383437	4.392061	-0.004002
C	-3.586821	3.736158	-0.003496
N	-4.690785	4.562001	-0.001491
C	-4.605857	5.936821	-0.000253
C	-3.414852	6.592421	-0.000907
C	-2.187373	5.790980	-0.002308
O	-3.704987	2.494075	-0.004166
H	-5.598990	4.103648	0.000689
O	-1.041821	6.247498	-0.002500
N	-1.449706	0.875216	0.027712
C	-0.186564	1.497658	0.004671
C	0.868732	0.533719	0.001795
C	0.519691	-0.829098	0.013890
N	-0.710899	-1.389323	0.029201
C	-1.678218	-0.479440	0.041792
N	2.243806	0.694334	-0.016368
C	2.715734	-0.536111	-0.015175
N	1.719472	-1.495303	0.001912
O	-0.109067	2.743841	-0.010975
N	-2.981800	-0.870052	0.120000
H	-2.274555	1.517206	0.032726
H	-3.709908	-0.204847	-0.126118
H	-3.173139	-1.848146	-0.073756
H	3.767384	-0.811845	-0.025823
H	1.844266	-2.504693	0.007110
H	-5.564952	6.455604	0.001239
C	-3.312303	8.092189	-0.000324
H	-1.518402	3.792840	-0.006415
H	-2.254646	8.386470	-0.002859
H	-3.794316	8.527634	-0.889047
H	-3.789690	8.526839	0.891290

TT1

C	-1.345643	-0.703451	-0.000379
C	-0.296219	-1.571226	0.000274
N	1.008735	-1.144111	0.000189
C	1.384692	0.195108	-0.000082
N	0.305458	1.065649	-0.000187
C	-1.046657	0.721408	-0.000513
O	2.559288	0.557876	-0.000138
O	-1.922755	1.608959	-0.000685
C	-2.777773	-1.140231	-0.000366
H	1.769054	-1.820148	0.000632
H	0.532464	2.085243	-0.000014
H	-3.304669	-0.747165	0.883422
H	-3.304735	-0.747348	-0.884202
H	-2.852516	-2.236679	-0.000282
H	-0.432417	-2.653220	0.001003
O	0.810227	3.847744	0.000290
C	-0.103017	4.690725	0.000111
N	0.158742	6.047271	-0.000020
C	-0.828599	7.006513	-0.000026
C	-2.152344	6.692343	-0.000019
C	-2.523085	5.274849	-0.000067
N	-1.439319	4.374198	0.000019
H	1.139363	6.318045	0.000277
H	-0.468018	8.035536	-0.000033
C	-3.237906	7.732240	-0.000007
O	-3.679314	4.841724	-0.000140
H	-1.663554	3.351399	-0.000085
H	-4.217432	7.235904	0.000409
H	-3.178022	8.377159	0.890048
H	-3.178545	8.376647	-0.890468

TT2

C	-1.403014	-0.804040	-0.000150
C	-0.347007	-1.663924	0.000558
N	0.954620	-1.227263	0.000535
C	1.320200	0.115748	-0.000137
N	0.234541	0.977521	-0.000720
C	-1.113569	0.622813	-0.000729
O	2.491997	0.486688	-0.000149
O	-1.996131	1.505169	-0.001135
C	-2.831118	-1.253767	-0.000077
H	1.720044	-1.897531	0.001002
H	0.453383	2.002958	-0.000918
H	-3.362566	-0.867021	0.883677
H	-3.362654	-0.867276	-0.883890
H	-2.895167	-2.350871	0.000079
H	-0.475801	-2.746850	0.001294
O	0.746440	3.728748	-0.000828
C	-0.132635	4.614647	-0.000410
C	0.163781	6.039962	0.000242
C	-0.888176	6.904960	0.000654
N	-2.191582	6.474560	0.000335
C	-2.563927	5.133734	-0.000298
N	-1.482729	4.265718	-0.000489
C	1.594444	6.482354	0.000486
H	-0.754542	7.987203	0.001259
H	-2.953761	7.148508	0.000782
O	-3.737797	4.769066	-0.000602
H	-1.706064	3.241450	-0.000697
H	1.664072	7.579312	0.000911
H	2.123473	6.091669	0.884146
H	2.123569	6.092337	-0.883407

TT3

C	-1.215203	-0.538902	0.000078
C	-0.260982	-1.507318	0.000294
N	1.084797	-1.213500	0.000310
C	1.580962	0.076157	0.000118
N	0.612716	1.052206	-0.000106
C	-0.782833	0.858769	-0.000122
O	2.800896	0.309543	0.000175
O	-1.543031	1.831135	-0.000299
C	-2.683461	-0.830916	0.000004
H	1.774479	-1.961539	0.000419
H	0.961365	2.036154	-0.000156
H	-3.167898	-0.385926	0.883541
H	-3.167798	-0.385780	-0.883511
H	-2.868624	-1.914111	-0.000087
H	-0.502610	-2.570531	0.000441

O	1.692352	3.657707	0.000057
C	2.910207	3.900849	0.000414
N	3.392753	5.194911	0.000951
C	4.734176	5.500798	0.001372
C	5.702537	4.545261	0.001262
C	5.283886	3.141569	0.000673
N	3.888432	2.935565	0.000331
H	2.695819	5.936045	0.000737
H	4.961317	6.567167	0.001820
C	7.168722	4.878700	0.001714
O	6.045205	2.169721	0.000457
H	3.550275	1.948908	0.000033
H	7.755782	3.950895	0.001165
H	7.447224	5.464650	-0.887760
H	7.446981	5.463408	0.892080

U-DAP

C	-0.168671	-1.498409	0.290778
C	1.139515	-1.306760	-0.020824
N	1.624602	-0.058166	-0.309035
C	0.836030	1.087783	-0.302150
N	-0.487289	0.873984	0.010392
C	-1.071135	-0.364323	0.313719
O	1.313843	2.200129	-0.558567
O	-2.284678	-0.435429	0.574221
H	-0.560855	-2.486484	0.518055
H	2.607268	0.075714	-0.536839
H	-1.121449	1.744136	0.022505
H	1.869391	-2.114848	-0.060812
N	-2.147686	3.164680	0.026332
C	-1.621690	4.405649	0.171837
C	-2.420725	5.569086	0.149514
C	-3.794784	5.415625	-0.025307
C	-4.353560	4.148294	-0.172697
C	-3.487192	3.032987	-0.142884
N	-0.267214	4.479294	0.392173
H	-1.961166	6.551293	0.265168
H	-4.439194	6.297466	-0.048482
H	-5.425921	4.004838	-0.310089
N	-3.960964	1.760012	-0.332112
H	0.306955	3.695088	0.057409
H	0.153586	5.395859	0.269862
H	-3.383201	0.977554	0.006673
H	-4.963891	1.633019	-0.236569

Coordinates of Contact ion-pair complexes

Z-1

C	8.592736	16.899448	17.149256
C	9.021926	16.875509	15.794116
C	10.201536	17.657629	15.688875
C	10.515477	18.164322	16.981455
C	9.510790	17.699491	17.884336
Zr	10.823316	15.724882	17.180415
F	12.177266	15.148803	15.379670
C	12.936002	15.723645	14.334550
C	13.097262	14.993113	13.167044
C	13.898789	15.648190	12.222685
C	14.455699	16.916984	12.430276
C	14.249280	17.586393	13.635180
C	13.475112	16.969204	14.617301
B	12.564056	13.422657	13.097975
C	10.949061	13.250863	13.400332
C	9.982567	14.256297	13.326475
C	8.606640	14.011664	13.387374
C	8.140497	12.710551	13.550262
C	9.064775	11.668226	13.629417
C	10.424854	11.957905	13.537826
F	14.198652	15.074134	11.040652
F	15.208602	17.495271	11.479266
F	14.790561	18.793939	13.854153
F	13.271726	17.569525	15.812902
F	10.334198	15.564895	13.179756
F	7.718322	15.029489	13.297342
F	6.821164	12.462732	13.628781
F	8.631379	10.401120	13.778907
F	11.267182	10.896479	13.572188
C	12.669047	12.746685	11.596993
C	13.209222	11.494346	11.291385
C	13.136525	10.914947	10.020010
C	12.484651	11.586845	8.989197
C	11.917907	12.835321	9.246701
C	12.014827	13.371378	10.528187
F	13.838008	10.746067	12.231885
F	11.425813	14.581625	10.721528
F	11.278650	13.497574	8.259967
F	12.396354	11.039608	7.762727
F	13.681903	9.702700	9.786444
C	13.555812	12.716969	14.215123
C	13.191890	12.255044	15.480333
C	14.096574	11.708462	16.396316
C	15.450331	11.644736	16.075637
C	15.872863	12.127731	14.836542
C	14.930714	12.654013	13.954435
F	11.903179	12.329434	15.914708
F	13.671681	11.263846	17.600964
F	16.335732	11.135508	16.949362
F	17.180172	12.085009	14.512291
F	15.405885	13.110328	12.769620
C	10.999096	15.426539	19.641317
C	11.949883	16.434442	19.296358
C	12.955745	15.832148	18.500770
C	12.638713	14.447026	18.365826
C	11.442194	14.193631	19.085971
C	9.334553	14.031898	17.093577
H	13.806557	16.342092	18.053454
H	11.899831	17.483597	19.574383
H	10.937117	13.236877	19.172301
H	10.101106	15.571780	20.237541
H	13.214656	13.715219	17.806759
H	9.455760	17.922165	18.946491
H	11.364079	18.794143	17.235386
H	10.775688	17.815487	14.778522
H	8.536683	16.343929	14.981880
H	7.725327	16.383819	17.551984
H	8.654656	13.974665	17.956959
H	8.724920	14.143067	16.183523
H	9.903968	13.089890	17.047520

Z-2

C	13.048223	6.904536	14.792561
C	12.709887	8.216202	14.358919
C	13.891146	9.009874	14.385447
C	14.956157	8.204311	14.864364
C	14.433034	6.896339	15.118604
Zr	13.396564	8.398986	16.784785
F	12.705918	10.563014	16.682620
C	13.137679	11.821849	17.182215
C	14.363603	12.289352	16.719275
C	14.769632	13.547850	17.160895
C	13.954041	14.297055	18.026010
C	12.725142	13.794675	18.467056
C	12.331210	12.489643	18.053452
F	15.140214	11.557052	15.891799
F	15.948597	14.043704	16.745763
F	14.426569	15.504535	18.390756
C	11.671119	14.377623	19.321086
C	10.611321	13.443689	19.483210
C	9.516303	13.778477	20.252668
C	9.410075	15.034455	20.857408
C	10.444258	15.957465	20.689210
C	11.571254	15.634834	19.924556
B	10.943471	12.039925	18.753208
C	11.068505	10.832672	19.830772
C	10.131044	9.802771	19.544891
C	9.970651	8.759142	20.462581
C	10.746910	8.718919	21.629663
C	11.688983	9.716615	21.892061
C	11.831871	10.765541	20.978374
F	12.521489	16.588738	19.806798
F	10.345433	17.173509	21.263275
F	8.332764	15.368570	21.593394
F	8.506147	12.889793	20.438353
C	9.441524	10.093605	18.270495
C	9.844353	11.368148	17.783688
C	9.353136	11.826703	16.578945
C	8.472718	11.058054	15.811030
C	8.091219	9.799032	16.278893
C	8.574086	9.313868	17.500851
F	8.180133	8.071545	17.859736
F	7.261416	9.038789	15.534725
F	8.000620	11.502963	14.629304
F	9.739118	13.035668	16.091428
F	12.748597	11.732072	21.252742
F	12.438572	9.653162	23.009469
F	10.587181	7.710556	22.509422
F	9.068578	7.766162	20.300035
C	14.316978	9.345126	18.932279
C	13.534085	8.222403	19.308776
C	14.142899	7.057269	18.768042
C	15.306798	7.462460	18.053555
C	15.410429	8.882478	18.144466
C	11.495297	7.279670	17.229697
H	11.718125	8.555917	14.066836
H	13.955057	10.066279	14.134680
H	14.999375	6.039197	15.472913
H	15.984931	8.523038	15.013925
H	12.364610	6.065396	14.881043
H	16.001209	6.806088	17.537133
H	16.190131	9.496998	17.699881
H	14.100168	10.381907	19.183280
H	12.610359	8.257966	19.877959
H	13.774098	6.039898	18.870966
H	10.767488	7.491361	16.428865
H	11.612465	6.187582	17.297316
H	11.102474	7.635845	18.194270

Z-3

C	8.037797	9.100873	18.337879
C	9.195793	8.265421	18.264078
C	9.845892	8.537296	17.029396
C	9.122829	9.558333	16.361024
C	7.995484	9.898499	17.162887
Zr	10.017334	10.602805	18.499518
C	9.369511	12.037989	20.473694
C	9.054669	10.690921	20.795970
C	10.280120	9.959751	20.891173
C	11.344594	10.870300	20.651067
C	10.786526	12.143871	20.369936
F	12.200560	9.647650	18.219264
B	12.812452	10.624874	17.302439
F	11.686233	11.566792	17.147787
F	13.870166	11.251336	17.915350
F	13.101410	10.029568	16.097963
C	9.095153	12.516198	17.647476
H	10.380876	8.903002	21.125533
H	12.400453	10.615424	20.607487
H	8.657905	12.842517	20.317718
H	11.341565	13.038576	20.096165
H	8.058328	10.291059	20.960432
H	9.397493	10.022719	15.416492
H	7.246896	10.646973	16.923392
H	9.512558	7.539122	19.008398
H	7.307801	9.111758	19.142021
H	10.782715	8.098517	16.694717
H	9.134621	12.437110	16.549639
H	8.056477	12.709773	17.952351
H	9.725146	13.357055	17.977680

Z-4

C	7.979701	9.137333	18.331438
C	9.134041	8.292899	18.305197
C	9.820948	8.537866	17.087252
C	9.122290	9.549895	16.377106
C	7.970989	9.906241	17.136223
Zr	9.952321	10.639109	18.506942

C	9.356639	12.062664	20.500577
C	9.006960	10.719835	20.805923
C	10.214193	9.956466	20.890315
C	11.300084	10.838903	20.650681
C	10.774630	12.130902	20.384058
F	12.172100	9.788110	18.140551
P	13.022993	10.853154	17.053109
F	11.527037	11.738447	17.085166
F	13.671307	11.938854	16.037595
F	12.412382	9.976103	15.809806
C	8.941512	12.532811	17.710626
H	10.288564	8.895600	21.114564
H	12.348622	10.558425	20.596999
H	8.664889	12.887340	20.361896
H	11.354066	13.011181	20.114278
H	8.000946	10.344311	20.970731
H	9.430628	9.994241	15.433379
H	7.229519	10.648531	16.859106
H	9.424829	7.579028	19.071515
H	7.227712	9.166984	19.114910
H	10.764590	8.090156	16.786653
H	8.948220	12.474120	16.611150
H	7.906588	12.678096	18.052542
H	9.547958	13.392434	18.036568
F	13.494021	11.716505	18.364331
F	14.341736	9.910017	17.136858

Z-5

C	12.931632	10.200220	15.243410
C	11.710512	10.376119	15.946945
C	11.922637	10.006418	17.302249
C	13.271020	9.572438	17.437554
C	13.899541	9.697083	16.168523
Zr	13.381003	12.031338	16.869813
F	10.989244	14.092888	12.122536
C	10.677759	14.819322	13.214165
C	10.960562	14.336947	14.495537
C	10.677860	15.047423	15.661991
C	10.044024	16.278975	15.462786
C	9.741892	16.802121	14.207456
C	10.061344	16.060310	13.068099
F	11.549450	13.106746	14.539320
B	10.888961	14.539191	17.194828
C	11.928707	15.374611	18.125089
C	12.175041	14.898483	19.420437
C	13.106395	15.463876	20.288685
C	13.834888	16.579385	19.871317
C	13.620698	17.096568	18.594265
C	12.686377	16.486505	17.750608
F	9.711524	17.028843	16.542035
F	9.148658	18.003126	14.077840
F	9.780133	16.539667	11.845056
F	11.486093	13.829993	19.887323
F	13.307413	14.954710	21.517876
F	14.734181	17.144256	20.691520
F	14.329672	18.164112	18.181459
F	12.577578	17.022654	16.510528
C	14.587446	13.064083	14.956105
C	15.557984	12.301692	15.672233
C	15.751289	12.913759	16.940317
C	14.909795	14.058965	17.005938
C	14.201349	14.158135	15.780720
F	11.547992	13.132179	17.154571
C	9.413539	14.285813	17.839207
C	8.601678	13.268724	17.324686
C	7.311211	13.004879	17.783824
C	6.775639	13.799936	18.798257
C	7.538522	14.840338	19.327948
C	8.829514	15.063990	18.842583
F	9.056689	12.485527	16.310619
F	6.576261	12.005315	17.255815
F	5.534043	13.568711	19.257522
F	7.023032	15.617947	20.300379
F	9.503511	16.097324	19.402149
C	13.932055	11.898838	19.062944
H	11.191792	10.076327	18.104839
H	10.793984	10.796414	15.540451
H	14.929567	9.437475	15.939080
H	13.100237	10.409036	14.189750
H	13.742180	9.228976	18.353578
H	14.213828	12.853094	13.957551
H	13.463046	14.915756	15.527524
H	14.803902	14.719185	17.862730
H	16.408924	12.562055	17.730391
H	16.061107	11.410709	15.307745
H	13.062700	11.487812	19.601643
H	14.803372	11.262190	19.277143
H	14.152825	12.912333	19.433370

Z-6

C	1.468027	4.911623	10.953332
C	1.688046	5.449521	9.681759
C	1.562276	6.842872	9.595883
C	1.201982	7.654489	10.668761
C	0.961067	7.068296	11.912212
C	1.096903	5.688829	12.054970
B	2.231087	4.604410	8.378849
C	1.490441	4.926615	6.951284
C	2.145564	4.581590	5.767972
C	1.606222	4.764028	4.497570
C	0.326361	5.306341	4.380795
C	-0.376772	5.652120	5.535096
C	0.207069	5.452614	6.790280
F	3.388995	4.022999	5.831461
F	2.299242	4.418132	3.391179
F	-0.224144	5.489069	3.169594
F	-1.614094	6.170983	5.426184
F	-0.538246	5.799352	7.862437
F	1.819325	7.466408	8.418575
F	1.112204	8.991409	10.530201
F	0.629797	7.829094	12.967060
F	0.894776	5.121296	13.257706
F	1.615093	3.586973	11.189385
C	3.686470	5.223831	8.298501
N	4.664523	5.843035	8.363828
B	5.879882	6.671110	8.838216
C	5.281956	7.432617	10.162916
C	5.070986	8.809370	10.282484
C	4.460166	9.393553	11.398107
C	4.032962	8.587949	12.451901
C	4.216822	7.205782	12.373838
C	4.819772	6.665762	11.240832
F	5.451764	9.665902	9.305004
F	4.280421	10.725296	11.462187
F	3.442600	9.132837	13.526204
F	3.801387	6.417599	13.383672
F	4.953414	5.314744	11.208753
C	6.415813	7.670278	7.663539
C	5.697914	8.025854	6.517969
C	6.181787	8.930713	5.567095
C	7.430611	9.524155	5.750782
C	8.179017	9.204478	6.885419
C	7.658491	8.297215	7.808275
F	4.464886	7.521231	6.285326
F	8.404068	8.064007	8.915833
F	9.379015	9.779442	7.078883
F	7.908243	10.394113	4.848117
F	5.452433	9.241005	4.479517
C	7.049381	5.549680	9.157732
C	7.332378	4.541232	8.251322
C	8.280747	3.540697	8.416519
C	9.046283	3.539177	9.580147
C	8.827637	4.539382	10.529504
C	7.853325	5.517497	10.303634
F	6.622377	4.489641	7.034974
Zr	7.223433	4.130224	4.797417
C	5.374432	2.741552	3.790228
C	5.705282	2.154373	5.041509
C	7.035435	1.643072	4.951626
C	7.526275	1.927298	3.650585
C	6.506518	2.623232	2.937358
F	8.485831	2.616009	7.453906
F	9.980812	2.601598	9.773920
F	9.565354	4.555063	11.648424
F	7.721483	6.456635	11.258154
C	2.254386	2.981737	8.533753
C	1.037394	2.305399	8.658879
C	0.933252	0.917694	8.730251
C	2.093859	0.143364	8.659489
C	3.329853	0.773912	8.524631
C	3.384050	2.168629	8.463507
F	-0.110798	3.019521	8.734929
F	-0.264208	0.317777	8.865424
F	2.019216	-1.197003	8.719170
F	4.456195	0.035633	8.446961
F	4.626073	2.713455	8.320583
C	8.660935	5.794792	3.587873
C	8.726367	6.163309	4.959649
C	9.383039	5.119747	5.665943
C	9.699679	4.086341	4.743659
C	9.256347	4.510078	3.452071
C	5.772775	5.618423	3.925525
H	8.317210	7.070054	5.397992
H	8.213240	6.378822	2.789088
H	9.366922	3.953928	2.525327
H	10.196727	3.147964	4.976505
H	7.580880	1.130826	5.739798
H	8.511325	1.668343	3.271331
H	6.577795	2.995627	1.917762
H	4.437455	3.229754	3.542539
H	5.062164	2.111931	5.917240
H	9.590927	5.109501	6.733933
H	4.806680	5.412749	4.418299
H	6.084683	6.647796	4.145615
H	5.614571	5.527305	2.841246

Z-7

C	15.973740	3.361602	6.192910
C	15.279895	2.472522	5.366852
C	16.046872	1.404579	4.892327
C	17.386418	1.207744	5.230162
C	18.022597	2.109458	6.082545
C	17.305253	3.199772	6.571677
B	13.713840	2.731228	4.981662
N	13.624784	3.890365	3.838259
B	14.753659	4.888079	3.214901
C	14.075779	5.456691	1.791571
C	12.780326	5.981424	1.797283
C	12.123789	6.503252	0.685634
C	12.798317	6.557193	-0.532391
C	14.106478	6.080418	-0.595517
C	14.716177	5.553182	0.548601
F	12.063980	6.017293	2.969347
F	10.855837	6.966718	0.779723
F	12.199022	7.062419	-1.622365
F	14.774069	6.133735	-1.762930
F	15.988283	5.130513	0.376115
F	15.523163	0.502858	4.022941
F	18.083675	0.178319	4.708704
F	19.316405	1.944316	6.402160
F	17.908452	4.094322	7.376872
F	15.343431	4.457240	6.684697
C	12.754734	3.112584	6.300680
C	11.443792	3.550361	6.132071
C	10.493107	3.659950	7.130539
C	10.820172	3.363991	8.446419
C	12.122480	2.935584	8.695868
C	13.041108	2.805285	7.643910
F	10.952331	3.885572	4.865525
Zr	8.579062	5.038790	4.573634
C	9.016352	6.955292	6.179705
C	10.061977	6.976361	5.211909
C	9.486587	7.259282	3.946307
C	8.077500	7.412985	4.132191
C	7.792847	7.239724	5.515701

F	14.244182	2.332712	8.017704
F	12.480623	2.630325	9.951503
F	9.917596	3.476093	9.426565
F	9.209306	4.024264	6.801981
C	8.755337	3.037819	3.065278
C	7.365697	3.262119	3.221461
C	7.056166	4.528332	2.647372
C	8.253317	5.065154	2.094425
C	9.309330	4.158122	2.369848
C	12.913737	1.367228	4.449126
C	12.944249	0.214069	5.248229
C	12.235247	-0.954993	4.976144
C	11.418579	-1.013428	3.846515
C	11.338255	0.103662	3.020564
C	12.073001	1.249192	3.338455
F	13.702131	0.200990	6.370501
F	12.320452	-2.020955	5.792675
F	10.718934	-2.122992	3.563607
F	10.547552	0.078232	1.929633
F	11.899242	2.287086	2.456030
C	16.076902	3.976281	2.912804
C	17.360231	4.169491	3.427345
C	18.447583	3.355958	3.098515
C	18.274367	2.285539	2.222833
C	17.006723	2.039759	1.695314
C	15.956219	2.879358	2.053845
F	17.614671	5.152426	4.325490
F	19.656652	3.568947	3.654152
F	19.308776	1.487014	1.913050
F	16.814832	1.001822	0.859458
F	14.740625	2.590505	1.501589
C	14.971990	6.261553	4.078424
C	15.874557	7.220010	3.597518
C	16.070905	8.469857	4.180392
C	15.310571	8.830751	5.293399
C	14.373286	7.929853	5.791312
C	14.218298	6.688935	5.170165
F	16.610494	6.945977	2.492587
F	16.967352	9.338076	3.674481
F	15.473480	10.034481	5.867862
F	13.609982	8.268817	6.851154
F	13.237280	5.897121	5.698823
H	12.822533	4.482212	4.054578
H	13.329806	3.393162	2.993523
C	6.676968	4.607106	5.740083
H	11.115338	6.782673	5.402693
H	9.130380	6.742580	7.240632
H	6.812489	7.296119	5.977726
H	7.353167	7.646661	3.356000
H	10.020618	7.340344	3.005641
H	9.305869	2.167081	3.414609
H	10.351222	4.283978	2.090463
H	8.349548	6.012867	1.572418
H	6.074285	4.994373	2.624330
H	6.664182	2.603870	3.724983
H	6.752801	5.037993	6.748903
H	5.759556	4.980841	5.262397
H	6.600880	3.508913	5.813813

Z-8

C	5.529996	-7.081797	17.130710
C	5.764852	-8.416663	16.690149
C	7.160522	-8.569037	16.472117
C	7.792973	-7.329745	16.797135
C	6.785377	-6.419580	17.215492
Zr	6.367932	-6.941099	14.772221
C	5.405768	-6.730262	12.437461
C	5.966603	-8.033651	12.540646
C	5.240710	-8.753808	13.527021
C	4.215647	-7.890794	14.028028
C	4.317244	-6.644175	13.348608
C	5.924080	-4.738044	14.932918
F	8.384083	-6.346585	13.833602
C	9.656444	-6.804577	13.444015
C	9.809541	-8.180028	13.433776
F	8.784436	-8.993040	13.777412
C	10.617307	-5.858097	13.129589
B	10.198925	-4.260908	13.150293
N	9.023696	-4.193078	12.158481
C	8.102513	-4.087023	11.448508
N	7.047286	-4.072438	10.723614
C	6.822238	-3.256959	9.752039
N	6.521869	-2.558149	8.869473
B	6.394566	-1.571814	7.681552
C	6.158182	-2.472370	6.324453
C	5.174771	-3.467979	6.333717
F	4.467924	-3.712871	7.469362
C	11.839426	-6.417211	12.743358
F	12.876740	-5.639193	12.381626
C	12.066640	-7.801075	12.706445
F	13.259104	-8.282330	12.325729
C	11.049929	-8.693338	13.052906
F	11.255035	-10.015330	13.016260
C	9.605554	-3.755929	14.605887
C	8.884901	-2.556817	14.671742
F	8.677844	-1.828862	13.547724
C	11.385185	-3.224655	12.722696
C	11.420409	-2.417750	11.582087
F	10.470421	-2.514026	10.616801
C	9.791303	-4.399514	15.830588
F	10.504385	-5.553806	15.911478
C	9.271436	-3.922394	17.036269
F	9.465803	-4.599138	18.186600
C	8.539007	-2.735936	17.047744
F	8.028213	-2.267647	18.197386
C	8.344328	-2.043327	15.852042
F	7.638732	-0.899162	15.850518
C	12.442918	-3.033628	13.618739
F	12.513112	-3.803741	14.734792
C	13.459320	-2.100276	13.431744
F	14.449449	-1.960572	14.333671
C	13.442957	-1.302574	12.286162
F	14.406747	-0.389968	12.083383
C	12.419884	-1.466056	11.353860
F	12.400536	-0.704002	10.245121
C	5.052765	-0.645913	7.827537
C	4.062772	-0.761150	8.804339
F	4.176438	-1.652322	9.823241
C	7.821121	-0.760379	7.759345
C	7.979903	0.569401	8.158020
F	6.911901	1.342709	8.471314
C	4.801991	0.309477	6.837076
F	5.714963	0.496187	5.851490
C	3.667901	1.117206	6.808353
F	3.491178	2.036730	5.838853
C	2.704597	0.967869	7.807322
F	1.597402	1.731726	7.802532
C	2.903664	0.021966	8.810241
F	1.974801	-0.130820	9.777024
C	9.017188	-1.452894	7.534336
F	8.977721	-2.768582	7.196134
C	10.281626	-0.875509	7.631714
F	11.394138	-1.593931	7.384781
C	10.387797	0.465760	8.002752
F	11.592770	1.050186	8.106153
C	9.228399	1.191233	8.268172
F	9.320763	2.483349	8.643197
C	6.785978	-2.271943	5.092435
F	7.739963	-1.323718	4.941626
C	6.481329	-3.019373	3.950624
F	7.120445	-2.790211	2.785450
C	5.503997	-4.011365	4.014999
F	5.199020	-4.738358	2.925337
C	4.843071	-4.240695	5.221364
F	3.889687	-5.192425	5.296290
H	8.860219	-7.123876	16.740447
H	7.657646	-9.467995	16.114694
H	5.008359	-9.180418	16.533720
H	4.562073	-6.644753	17.366026
H	6.936859	-5.389483	17.523165
H	3.476244	-8.147410	14.782348
H	5.429012	-9.776846	13.843932
H	6.826819	-8.405652	11.987301
H	5.755021	-5.932278	11.784059
H	3.688052	-5.773702	13.510261
H	5.047469	-4.472560	15.542509
H	6.811765	-4.296291	15.418584
H	5.797054	-4.299880	13.931024

Coordinates of newly designed planar cationic AAAA-DDDD molecules

A-1

C	0.025239	18.039578	20.704515
C	0.426322	17.888001	19.375360
C	1.351575	18.771742	18.754410
C	1.894719	19.841283	19.477514
C	1.495884	19.996588	20.807856
C	0.577416	19.111960	21.411558
N	1.562907	18.378626	17.437183
C	0.792126	17.305373	17.288839
N	0.089715	16.960151	18.404392
N	0.660222	16.546789	16.131644
C	1.318857	16.827715	14.971508
N	2.134955	17.865036	14.882102
N	1.099619	15.997452	13.915537
C	1.711022	16.171133	12.677699
N	1.447646	15.310728	11.653827
C	2.207524	15.747381	10.581712
C	2.905677	16.896287	11.045170
N	2.571720	17.140019	12.371099
C	3.774826	17.585740	10.189950
C	3.922724	17.103314	8.887104
C	3.223386	15.962712	8.438501
C	2.351917	15.263261	9.278884
N	-0.138179	13.114398	11.828352
B	-0.797908	12.844119	13.088411
N	-1.656048	11.603360	13.181504
C	-1.771437	10.722667	12.068895
C	-1.079710	11.085150	10.886739
C	-0.290557	12.291209	10.835861
C	-1.168353	10.242568	9.760539
C	-1.912492	9.077395	9.805519
C	-2.602272	8.702023	10.981575
C	-2.520578	9.536610	12.100431
C	-3.404362	7.401765	10.992669
C	-2.447833	6.226421	10.694115
C	-2.296852	11.375356	14.339344
C	-2.163358	12.236900	15.429618
C	-2.855978	11.963862	16.623823
C	-2.722181	12.810400	17.709225
C	-1.841514	13.951579	17.543721
N	-1.639181	14.835066	18.583656
C	-2.250243	14.639739	19.728761
C	-3.140372	13.561932	20.010642
C	-3.397457	12.611734	18.982777
C	-3.759425	13.424449	21.269086
C	-4.621803	12.365452	21.507828
C	-4.897014	11.409700	20.501848
C	-4.275637	11.552521	19.254382
N	-0.657756	13.707482	14.205402
C	-1.309857	13.415958	15.334653
N	-1.174438	14.237121	16.415513
C	-5.848106	10.234045	20.730017
C	-5.081493	8.912785	20.505843
C	-6.439589	10.219861	22.146619
C	-7.008601	10.323321	19.715058
C	-4.095527	7.140463	12.337722
C	-4.482395	7.470095	9.889643
H	0.811162	14.445952	11.698162
H	0.443939	15.170887	14.039965
H	4.316580	18.468000	10.535653
H	4.594555	17.619358	8.198649
H	3.366082	15.618895	7.412430
H	1.812047	14.381521	8.927345
H	2.252232	18.444275	15.733482

H	2.602671	18.007937	13.966232
H	0.016304	15.718818	16.177189
H	-0.581638	16.141709	18.474744
H	-0.684499	17.356526	21.175758
H	0.291284	19.267920	22.453268
H	1.902928	20.821362	21.395719
H	2.604987	20.526962	19.012278
H	-2.049625	15.372328	20.520353
H	-3.551888	14.159961	22.049691
H	-5.091737	12.273763	22.486244
H	-4.490251	10.814601	18.480286
H	-3.491279	11.077128	16.671020
H	-2.937924	10.499178	14.431776
H	-3.052992	9.238675	13.000802
H	-1.965950	8.438313	8.923445
H	-0.633699	10.528021	8.851867
H	0.211982	12.507404	9.880085
H	-7.110784	9.354090	22.244281
H	-7.025910	11.129232	22.349512
H	-5.653823	10.128598	22.912403
H	-6.640864	10.286395	18.678580
H	-7.576739	11.256104	19.850941
H	-7.690257	9.472781	19.868224
H	-4.679390	8.848147	19.483769
H	-5.767008	8.065129	20.659133
H	-4.246135	8.819510	21.216466
H	-4.810458	7.940062	12.587633
H	-3.365207	7.046728	13.156972
H	-4.653927	6.195112	12.274881
H	-5.181456	8.299393	10.076501
H	-5.051116	6.527622	9.879741
H	-4.033087	7.608541	8.895319
H	-1.666517	6.151561	11.466179
H	-1.961372	6.342943	9.714595
H	-3.020189	5.286107	10.683445

A-2

C	-2.536098	9.523921	12.109291
C	-1.787702	10.716304	12.092154
C	-1.100024	11.069431	10.901922
C	-1.176619	10.235343	9.766204
C	-1.919450	9.070693	9.813432
C	-2.613467	8.691687	10.990312
C	-1.661358	11.626325	13.223845
C	-0.827049	12.824105	13.101742
N	-0.192714	13.094342	11.898019
C	-0.331006	12.273592	10.887295
C	-2.307835	11.399885	14.418961
N	-2.166948	12.257451	15.472489
B	-1.286154	13.464020	15.341250
N	-0.637850	13.687077	14.088038
N	-1.149037	14.319852	16.477461
C	-1.806804	14.027235	17.588164
C	-2.686031	12.863523	17.725067
C	-2.823066	12.017954	16.647357
C	-3.381078	12.628572	18.986556
C	-3.144667	13.558672	20.035787
C	-2.258075	14.653283	19.792973
N	-1.633710	14.884515	18.666151
C	-3.778905	13.393169	21.281689
C	-4.638568	12.324752	21.490466
C	-4.893394	11.388276	20.463635
C	-4.255776	11.559022	19.227375
C	-5.840821	10.203477	20.654267
C	-6.451271	10.159270	22.061773
C	-3.411646	7.389420	10.992008
C	-4.108688	7.121790	12.332964
C	-6.987071	10.309084	19.625024
C	-5.062851	8.891675	20.415022
C	-4.485156	7.456684	9.884637
C	-2.451238	6.216991	10.694781
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D-1

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D-2

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D-3

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H	1.662125	2.247957	18.784045
H	0.169463	1.267933	18.938051
H	-3.371477	-0.928294	17.560729
H	-4.131803	0.028851	18.854724
H	-5.876856	-0.950686	17.323125
H	-5.894566	0.832290	17.229337
H	-5.128886	-0.121370	15.928582
H	0.190112	6.501827	15.280226
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H	0.159294	2.158910	14.770036
H	0.198198	0.743930	12.716615
H	-1.957889	0.092524	11.610777

H	-4.136657	2.282342	14.629089
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H	5.507048	9.686919	15.415746
H	7.913256	10.161334	15.919793
H	9.195580	8.561651	17.351313
H	8.151292	6.566114	18.253473
H	5.643846	-0.023608	21.588678
H	8.036696	0.308287	22.245969
H	8.170912	3.954410	19.984430
H	9.260514	2.322574	21.410977

D-4

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C	1.147821	15.926468	11.876892
C	0.325250	14.728773	11.891192
C	0.658672	16.997463	15.313703
N	0.058595	16.609291	16.467060
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N	-0.849975	14.518143	15.380092
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C	1.803990	16.320693	10.701190
C	2.369503	20.884988	20.890943
C	1.733297	22.282739	21.052190
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C	2.930389	20.646037	12.288546
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E-1

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C	-0.047921	19.019535	21.652922
C	0.870555	19.926427	21.068490
C	1.070672	18.656387	17.532980
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C	-0.260777	16.749834	17.274110
C	-0.711894	16.806886	18.645946
C	-1.622474	15.844791	19.057716
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H	1.958299	20.528185	19.323407
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H	-8.220842	12.194605	20.009420
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H	1.572159	19.870914	23.714708

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E-2

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C	1.224499	-0.040106	-0.669692
N	0.962011	0.044039	3.481059
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N	0.131616	-0.378568	8.779469
C	0.942869	-0.740342	11.141284
C	0.546698	-0.658766	12.476760
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H	-9.722300	6.430451	10.312960
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E-3

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N	2.236309	17.648048	17.571651
C	1.278505	16.742873	17.423315
N	0.747872	16.280102	18.597654
N	0.821237	16.237323	16.217118
C	1.210925	16.718240	15.004629
N	2.012708	17.764235	14.895322
Br	0.144205	15.720277	21.881258
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C	0.991010	16.461720	12.608390
N	0.582697	15.674950	11.564626
C	0.982432	16.340190	10.418482
C	1.615526	17.537984	10.859584
N	1.600682	17.582636	12.246915
C	2.130018	18.457295	9.938381
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C	-5.256534	13.081768	21.219879
C	-5.485756	12.038413	20.292478
C	-4.723137	12.008446	19.118026
C	-2.529409	6.981237	11.083759
C	-1.477858	5.858310	10.955632
C	-6.536590	10.951855	20.526014
C	-5.848279	9.570003	20.505268
C	-7.263609	11.113147	21.868369
C	-7.580667	11.014660	19.390459
C	-3.384094	6.709585	12.329369
C	-3.448548	6.959957	9.843383
H	0.330690	14.656708	11.684567
H	0.214271	15.150824	14.048841
H	2.613441	19.374503	10.276911
H	2.388071	18.853473	7.834808
H	1.262998	16.787938	7.068555
H	2.387492	18.164204	15.771812
H	2.215819	18.103620	13.940117
H	0.075143	15.486368	16.253999
H	-0.172163	15.764929	18.643953
H	2.161884	17.723338	22.820497
H	3.766851	19.221935	21.680221
H	3.923112	19.287065	19.178655
H	-2.317924	15.751502	20.288607
H	-4.126269	14.857081	21.699780
H	-5.836628	13.125546	22.140887
H	-4.904043	11.207166	18.400835
H	-3.656952	11.177210	16.732629
H	-2.811149	10.317990	14.569938
H	-2.592669	8.920224	13.054066
H	-0.857773	8.036609	9.213319
H	0.322780	10.214194	9.222590
H	0.764277	12.386944	10.294516
H	-7.996006	10.299725	21.977359
H	-7.805630	12.069593	21.922788
H	-6.563637	11.056279	22.716343
H	-7.114861	10.856091	18.406226
H	-8.090667	11.990100	19.381361
H	-8.334438	10.227313	19.545292
H	-5.353215	9.379843	19.541230
H	-6.603483	8.784922	20.663675
H	-5.094843	9.495939	21.304497
H	-4.174151	7.467096	12.450583
H	-2.770641	6.688362	13.243659
H	-3.868952	5.727951	12.223003
H	-4.217089	7.745406	9.913171
H	-3.952149	5.982965	9.780811
H	-2.877436	7.112189	8.915827
H	-0.812523	5.843922	11.832651
H	-0.862933	5.981931	10.052372
H	-1.990624	4.886247	10.890702

E-4

C	-4.430398	11.766700	19.291910
C	-3.465481	12.745825	19.010420
C	-3.149713	13.701021	20.016238
C	-3.794929	13.642820	21.267360
C	-4.740987	12.660296	21.518735
C	-5.078642	11.704763	20.531891
C	-2.168113	14.696986	19.727017
N	-1.538843	14.820476	18.581359
C	-1.812812	13.936840	17.557493
C	-2.756025	12.853078	17.744608
C	-2.905298	11.958200	16.697674
C	-2.195951	12.150127	15.499411
C	-1.337162	13.305788	15.375568
N	-1.146323	14.158285	16.413166

C	-2.290052	11.256953	14.419201
C	-1.588331	11.503684	13.249422
C	-0.814348	12.727368	13.190112
N	-0.686338	13.581714	14.218653
C	-1.603637	10.621968	12.093745
C	-0.875865	11.039314	10.948224
C	-0.189657	12.290112	10.993755
N	-0.151627	13.088264	12.036088
C	-0.852482	10.226082	9.793712
C	-1.535259	9.024476	9.781673
C	-2.268553	8.583652	10.914141
C	-2.289605	9.392390	12.051617
C	-2.999830	7.244102	10.846294
C	-4.017855	7.286558	9.686620
C	-6.128911	10.618869	20.771697
C	-7.272647	10.797427	19.750116
C	-1.969050	6.126581	10.575425
C	-3.750542	6.912767	12.143192
C	-5.481455	9.232426	20.568990
C	-6.724117	10.676863	22.185599
N	0.903345	15.585740	11.578180
C	1.245841	16.412586	12.604653
N	1.932938	17.489157	12.237081
C	2.068061	17.358719	10.858581
C	1.431270	16.165709	10.437932
C	2.703455	18.196354	9.927456
C	2.676696	17.797021	8.593018
C	2.042711	16.605604	8.171028
C	1.405166	15.767523	9.092692
N	0.869503	16.089272	13.904096
C	1.273983	16.793965	14.996046
N	2.063905	17.848918	14.884151
O	0.756769	14.594261	8.804861
C	0.712258	14.207936	7.421900
N	0.828723	16.364194	16.208286
C	1.172931	16.976077	17.408994
N	2.051462	17.962154	17.557729
C	2.043455	18.228789	18.923056
C	1.127453	17.358967	19.563186
N	0.591275	16.560635	18.568179
C	2.773272	19.170876	19.666194
C	2.551052	19.204656	21.041135
C	1.635949	18.337959	21.682284
C	0.906999	17.395478	20.948475
O	-0.001977	16.503376	21.455890
C	-0.215021	16.540637	22.875961
H	0.474540	14.624731	11.709696
H	0.307153	15.213190	14.041049
H	3.194949	19.117874	10.241226
H	3.159694	18.418660	7.837007
H	2.054855	16.345133	7.113242
H	2.361473	18.306229	15.764884
H	2.334773	18.130549	13.924555
H	0.141418	15.571668	16.250286
H	-0.219432	15.878590	18.615834
H	1.504713	18.410105	22.761500
H	3.097939	19.921964	21.655714
H	3.482181	19.843647	19.182583
H	-1.891465	15.418314	20.503961
H	-3.543644	14.380147	22.033289
H	-5.229253	12.630313	22.492071
H	-4.694750	11.033152	18.529348
H	-3.564132	11.091886	16.781682
H	-2.925256	10.375412	14.523336
H	-2.845214	9.058422	12.926764
H	-1.509857	8.402238	8.886165
H	-0.288652	10.556853	8.918558
H	0.344096	12.641868	10.103614
H	-7.466763	9.872801	22.293724
H	-7.231794	11.635888	22.371354
H	-5.951007	10.532207	22.955872
H	-6.904694	10.716606	18.716210
H	-7.756799	11.778454	19.872150
H	-8.028355	10.012679	19.909087
H	-5.083295	9.117980	19.549595
H	-6.238817	8.449878	20.730526
H	-4.659676	9.076152	21.284211
H	-4.519215	7.668247	12.368820
H	-3.063733	6.839378	13.000964
H	-4.252435	5.940761	12.027474
H	-4.768006	8.074478	9.854215
H	-4.536556	6.317534	9.622890
H	-3.523574	7.474127	8.722045
H	-1.228883	6.071736	11.388718
H	-1.434966	6.292441	9.628261
H	-2.490079	5.158899	10.511570
H	-0.956276	15.760621	23.088083
H	0.719487	16.323415	23.418451
H	-0.603449	17.523339	23.189733
H	0.149807	13.266917	7.391847
H	0.193969	14.970949	6.818480
H	1.728293	14.050777	7.024054

Coordinates of complexes of designed anions with zirconocene cation

12a

C	-0.055788	0.416429	-0.253904
C	-0.107255	0.433415	1.169367
C	1.152274	0.585162	1.826778
C	2.311769	0.868163	1.082749
C	2.331676	1.010368	-0.300707
C	1.121693	0.760139	-0.941243
B	-1.551467	0.594940	2.046724
N	-1.213458	1.816717	2.961192
C	-0.949523	2.758337	3.600235
N	-0.801088	3.790266	4.332926
C	0.236106	4.418758	4.707573
N	1.111829	5.062648	5.143370
B	2.305277	5.882271	5.729225
C	1.625119	6.430822	7.191384
C	0.272791	6.889243	7.222910
C	-0.434054	6.932011	8.438311
C	0.095926	6.533522	9.663066
C	1.439874	6.178595	9.637381
C	2.219563	6.192151	8.467463
C	-0.617894	7.327450	6.047274
F	-1.655809	6.448592	5.891659
F	-1.720023	7.319684	8.445100
C	-0.799910	6.539941	10.891037
F	-1.907343	5.777134	10.682285
F	2.003926	5.754570	10.785064
C	3.689378	5.884595	8.754840
F	4.147112	6.637704	9.791460
C	1.465641	0.518045	3.324814
F	2.448825	-0.385246	3.570752
F	3.480056	1.067303	1.722818
C	3.628880	1.411397	-0.981663
F	4.597547	0.481254	-0.752696
F	1.075016	0.890807	-2.275544
C	-1.205334	0.092157	-1.211686
F	-1.633924	1.213550	-1.865954
C	-2.893522	1.217300	1.205043
C	-2.893688	2.563871	0.729909
C	-4.103483	3.216572	0.406198
C	-5.349177	2.611476	0.512525
C	-5.329260	1.272744	0.899007
C	-4.157919	0.555682	1.169135
C	-1.694885	3.504178	0.524365
F	-0.468962	2.968509	0.699953
C	-4.422990	-0.921334	1.451265
F	-4.996213	-1.096028	2.682545
F	-6.524911	0.673839	1.047384
C	-6.685019	3.281522	0.245689
F	-7.462101	3.259625	1.364608
F	-4.061496	4.501327	0.020238
C	-1.829642	-0.626204	3.205527
C	-1.163363	-1.889946	3.171204
C	-1.013220	-2.646547	4.339680
C	-1.585813	-2.310782	5.565556
C	-2.375741	-1.167762	5.553810
C	-2.514231	-0.334970	4.423145
C	-0.519288	-2.565009	1.958806
F	-0.858278	-2.045788	0.767997
F	-0.249559	-3.753907	4.320869
C	-1.348309	-3.213910	6.762238
F	-0.012283	-3.384555	6.979635
F	-2.997338	-0.821229	6.694161
C	-3.422560	0.863431	4.722430
F	-3.731091	1.655637	3.677757
F	0.846470	-2.532157	2.043798
F	-0.886549	-3.877103	1.891165
F	-1.877362	-2.745757	7.911342
F	-1.878080	-4.449053	6.544883
F	-4.615073	0.452878	5.227773
F	-2.840577	1.681869	5.665898
F	-5.281929	-1.447008	0.532669
F	-3.334849	-1.710253	1.402509
F	-6.583737	4.568973	-0.143208
F	-7.364469	2.619149	-0.731283
F	-1.689347	4.000348	-0.742694
F	-1.764528	4.570402	1.383016
C	2.541484	7.046339	4.514621
C	2.566053	8.447036	4.781567
C	2.244948	9.368540	3.775827
C	1.982580	9.016499	2.453205
C	2.109309	7.662630	2.163513
C	2.409115	6.689427	3.139104
C	2.859761	9.119467	6.120251
F	3.407674	8.317263	7.052478
F	2.128831	10.672381	4.085281
C	1.586205	10.099536	1.464267
F	2.564851	11.041098	1.364331
F	1.890395	7.261159	0.902250
C	2.520766	5.291174	2.520599
F	1.311563	4.859380	2.039858
C	3.470607	4.650638	5.887093
C	4.780720	4.720231	5.340801
C	5.525815	3.555359	5.080191
C	5.114939	2.282194	5.470426
C	3.889020	2.229461	6.117259
C	3.074282	3.353634	6.345580
C	5.506686	5.994553	4.897481
F	4.990880	7.133365	5.388299
F	6.665479	3.659667	4.387995
C	5.885856	0.990519	5.245421
F	5.170121	0.139531	4.465910
F	3.462856	1.011456	6.512055
C	1.802299	2.974702	7.062059
F	1.055114	2.066388	6.412304
F	3.748369	10.140746	5.963354
F	1.722887	9.650153	6.665780
F	1.347874	9.637135	0.220259
F	0.455640	10.734654	1.882323
F	3.391176	5.292054	1.476980
F	2.961577	4.319230	3.349803
F	6.802757	5.981219	5.317416
F	5.517929	6.100185	3.536693
F	2.210576	2.290935	8.315375
F	0.982960	3.907810	7.518049
F	7.083962	1.172132	4.660026
F	6.108854	0.365217	6.436761
F	-1.149384	8.555116	6.287524
F	-0.024218	7.424397	4.840949
F	-0.195927	6.067434	12.003322
F	-1.222083	7.803498	11.164797
F	3.853826	4.563878	9.115680
F	4.536511	6.119607	7.741894
F	1.915714	1.741471	3.771588
F	0.457315	0.179669	4.159854
F	3.519238	1.552691	-2.317997
F	4.080729	2.596581	-0.486393
F	-0.796051	-0.799962	-2.160015
F	-2.287009	-0.471349	-0.645610

Zr	1.138617	1.099239	9.966361
C	-0.282489	2.777370	10.452926
C	0.518160	-0.431948	8.066301
C	1.771315	1.733834	12.309132
C	1.866105	0.316849	12.192572
C	2.936327	0.016930	11.293473
C	3.489236	1.248188	10.853656
C	2.763838	2.308191	11.469448
H	2.928267	3.371631	11.308776
H	4.305702	1.363502	10.142444
H	3.267971	-0.975857	11.000957
H	1.255221	-0.410454	12.721189
C	0.761432	-1.234247	9.211188
C	-0.249542	-0.936230	10.174959
C	-1.117314	0.044493	9.616333
C	-0.634182	0.366278	8.320298
H	-1.076888	1.092984	7.643538
H	-1.986787	0.481827	10.098393
H	-0.357776	-1.403976	11.149778
H	1.564969	-1.956561	9.326424
H	-0.994655	2.573104	11.265883
H	0.309842	3.658507	10.747235
H	-0.873068	3.000204	9.547777
H	1.126890	-0.415982	7.164370
H	1.052513	2.279184	12.913753

12b

C	0.268884	-3.122669	15.852181
N	0.989816	-4.233170	16.312455
C	0.423631	-4.581861	17.542237
C	-0.649364	-3.737418	17.814915
C	-0.698370	-2.770409	16.780924
B	2.314399	-4.734462	15.593882
N	3.392244	-5.443234	16.498404
C	3.851010	-6.743662	16.329055
C	5.140523	-6.852669	16.833695
C	5.462410	-5.597888	17.421059
C	4.365618	-4.769358	17.223690
C	2.931266	-7.901508	15.996445
F	3.111147	-8.420827	14.756810
C	6.077833	-8.025120	16.683271
F	5.517317	-9.071981	16.034217
C	6.693707	-5.247407	18.220197
F	7.040543	-3.941178	18.060822
C	4.177497	-3.402242	17.841837
F	2.872744	-3.021986	17.868833
C	0.807830	-5.688743	18.520308
F	2.096198	-6.087384	18.494109
C	-1.697699	-3.871509	18.901415
F	-2.894453	-3.394693	18.462314
C	-1.547465	-1.517533	16.783975
F	-2.762672	-1.693283	16.208537
C	0.366566	-2.446333	14.496770
F	0.919579	-3.213866	13.525783
N	2.999189	-3.428338	15.134582
C	3.524273	-2.475361	14.710549
N	4.173811	-1.454952	14.331287
C	4.013359	-0.590146	13.428786
N	3.986840	0.269177	12.629943
B	3.838153	1.102892	11.350971
N	3.577815	2.595982	11.888227
C	4.279405	3.745239	11.540673
C	4.230315	4.675140	12.578097
C	3.439320	4.095984	13.605176
C	3.022157	2.852923	13.138747
C	4.947715	4.018788	10.242454
F	4.672939	3.232346	9.221499
C	4.842101	6.062185	12.559129
F	4.087861	6.928092	11.838037
C	3.206361	4.717308	14.967654
F	2.431553	3.976309	15.782763
C	1.965116	1.992859	13.825025
F	2.454293	1.399508	14.947034
N	5.229527	0.968525	10.572414
C	6.415559	0.712907	11.269676
C	7.326588	0.077145	10.440860
C	6.731077	0.000510	9.151657
C	5.452421	0.537616	9.257948
C	6.743482	1.169460	12.680111
F	6.699314	0.170295	13.596342
C	4.545876	0.704905	8.041038
F	3.319405	1.204745	8.279298
C	7.429608	-0.590116	7.940967
F	8.744395	-0.235035	7.936262
C	8.680613	-0.471984	10.839561
F	8.970735	-1.606717	10.163920
N	2.621209	0.452470	10.590068
C	2.433302	-0.926508	10.450317
C	1.093240	-1.188779	10.184034
C	0.418846	0.060589	10.185084
C	1.380400	1.043324	10.363079
C	3.484616	-2.024223	10.516160
F	3.056164	-3.000948	11.371846
C	0.428323	-2.514463	9.870341
F	-0.540745	-2.341385	8.931626
C	-1.080899	0.264147	10.162951
F	-1.583913	0.410009	8.912361
C	1.111267	2.523325	10.165921
F	0.110801	2.691390	9.270740
N	2.073030	-5.589766	14.270761
C	0.856051	-5.957890	13.692378
C	1.060146	-6.320066	12.366696
C	2.459285	-6.285601	12.132341
C	3.054411	-5.799801	13.291467
C	-0.512841	-6.069362	14.353355
F	-1.264976	-4.946106	14.175319
C	0.000537	-6.556481	11.308618
F	-1.133372	-5.851398	11.557863
C	3.132170	-6.798645	10.873806
F	3.278575	-5.824721	9.937947
C	4.566508	-5.639543	13.404757
F	5.180066	-6.837675	13.574588
F	-1.189534	-7.106078	13.795814
F	-0.492661	-6.324372	15.676057
F	0.437638	-6.128441	10.095358
F	-0.345112	-7.864122	11.185274
F	4.360586	-7.323946	11.107057
F	2.403995	-7.803962	10.317389
F	5.042946	-5.082013	12.259302
F	5.014387	-4.845639	14.409064
F	5.121596	1.559572	7.148400
F	4.374065	-0.492222	7.428658
F	7.361547	-1.947437	7.963544
F	6.929254	-0.186642	6.754723
F	9.684180	0.422360	10.596683
F	8.735273	-0.789205	12.155762
F	8.002199	1.686613	12.706402
F	5.928641	2.157073	13.129176
F	3.698717	-2.579726	9.306487
F	4.708857	-1.646704	10.969147
F	0.748988	3.170464	11.307934
F	2.178256	3.186037	9.653479
F	-1.713524	-0.786086	10.744387
F	-1.437528	1.361612	10.884465
F	1.284762	-3.432104	9.372041
F	-0.151846	-3.061420	10.969563
F	4.778753	5.282033	9.839804
F	6.414703	3.879184	10.414292
F	5.007538	6.589390	13.781119
F	6.099560	6.047562	11.987359
F	4.396334	4.874316	15.611491
F	2.623863	5.940025	14.851681
F	0.903790	2.750136	14.172626
F	1.475982	1.008562	13.034186
F	3.104883	-8.904312	16.893807
F	1.630834	-7.534045	16.098996
F	7.167866	-7.666832	15.949547
F	6.520586	-8.478417	17.886782
F	6.489679	-5.455861	19.551843
F	7.770783	-5.983316	17.866661
F	4.606671	-3.403330	19.124233
F	4.862612	-2.420003	17.187828
F	0.601808	-5.235395	19.787980
F	0.048225	-6.798271	18.345939
F	-1.925316	-5.163156	19.247853
F	-1.375838	-3.189649	20.031092
F	-1.748260	-1.081678	18.056670
F	-0.933029	-0.492064	16.134693
F	-0.859406	-2.097688	14.054145
F	1.114105	-1.293147	14.541616
Zr	8.332024	5.064712	9.706109
C	8.807377	3.224623	8.496182
C	6.981048	6.989630	8.808576
C	9.829773	3.801062	11.327391
H	9.743829	3.254475	7.920101
H	8.875202	2.372590	9.190677
H	7.979758	3.061311	7.785289
C	8.317925	7.436834	8.936963
C	9.120269	6.691649	8.017101
C	8.266514	5.802897	7.305822
C	6.947957	5.968128	7.809556
H	6.066376	5.422938	7.478390
H	8.573001	5.105621	6.532413
H	10.192028	6.801377	7.868831
H	8.672213	8.199517	9.625453
C	10.667636	4.620340	10.521767
C	10.356984	5.980029	10.806817
C	9.304920	6.001546	11.768324
C	8.987912	4.648556	12.093363
H	8.224457	4.324425	12.797282
H	8.836922	6.889801	12.186611
H	10.832745	6.850295	10.364362
H	11.412730	4.267080	9.813655
H	6.135717	7.348702	9.391532
H	9.824212	2.716033	11.332671