Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for:

Substituent Effects in Cation/π Interactions Revisited: A General Approach from Intrinsic Properties of the Arenes

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Contents of Supplementary Information:

1. Computational details

The geometry of the arenes and the interaction energies and equilibrium distances of all 171 cation/π complexes were obtained at the M06-2X/6-31+G* level following the same procedure as Wheeler and Houk,[1] i.e., by scanning the distance between Na^+ and the center of mass of the atoms forming the ring at 0.05 Å increments with the geometry of the substituted aromatics frozen. The excellent linear correlation (y=0.99x-0.55, r^2=0.9980) obtained for our interaction energies with Wheeler's and Houk's (computed at the M05-2X/6-311+G(2df,2p) level and nicely correlated with those computed at the CCSD(T)/aug-cc-pVTZ level, r^2=0.9998) indicates that the M06-2X/6-31+G* level of theory is an excellent choice to study cation/π interactions. Other geometries, e.g., cation-dipole arrangements (important for monosubstituted benzenes) were not considered because our study is devoted to the nature of the cation-π interaction and not to the nature of the cation-dipole interaction. We used the same set of substituents as Wheeler and Houk with the addition of X=Cl, Br and NC. In all cases, the lowest-energy conformation was utilized and the cation located above the face of the ring that yields the lowest energy. These lowest-energy conformations were confirmed to be minima on the potential energy surface by performing vibrational frequency calculations. The reported interaction energy is the minimum energy obtained along these rigid-monomer scans. The Θ_{zz} and α_{zz} were computed at the same level of theory, which are in excellent agreement with the experimental results: calculated/experimental Θ_{zz} (B) for benzene = -8.6/-8.5,[2] fluorobenzene = -6.2/-6.3,[3] 1,3,5-trifluorobenzene = 0.6/0.9,[4] hexafluorobenzene = 9.1/9.5, 1,3,5-trichlorobenzene = -3.3/-3.2,[5] and calculated/experimental isotropic polarizabilities $\langle\alpha\rangle$ (a.u.) for benzene = 63.8/63.8,[6] toluene = 76.4/79.6, fluorobenzene = 63.8/69.5,[7] phenol = 73.2/74.9, cyanobenzene = 80.7/84.3, *p*-xylene = 89.2/92.5, 1,3,5-trimethylbenzene = 101.8/104.6, and hexamethylbenzene = 137.1/141.0. The zz component of the atomic dipole polarizability tensor was calculated as the set of first derivatives of the atomic

[1] S. E. Wheeler, K. N. Houk, *J. Am. Chem. Soc.* 2009, **131**, 3126.
[2] G. R. Dennis, G. L. D. Ritchie, *J. Phys. Chem.*, 1991, **95**, 656.
[3] G. R. Dennis, I. R. Gentle, G. L. D. Ritchie, *J. Chem. Soc., Faraday Trans. 2*, 1983, **79**, 529.
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[5] G. L. D. Ritchie, *Chem. Phys. Lett.* 1982, **93**, 410.
[6] M. J. Aroney, S. J. Pratten, *J. Chem. Soc., Faraday Trans. 1*, 1984, **80,** 1201.
[7] A. A. Maryott, F. Buckley, *U. S. National Bureau of Standards Circular No. 537*, 1953.

z dipole moment component with respect to the z component of an applied electric field of 0.0025 a.u. along the z direction, the derivatives being evaluated at the zero-field point. BSSE correction was not taken into account because, when relatively small basis sets are used, its inclusion is not recommended in the calculation of interaction energies since it would lead to values with larger discrepancies with the ones calculated by means of extrapolation to the basis set limit.[8] All calculations were carried out with Gaussian09 package,[9] apart from the Θ_{zz} and the atomic dipole polarizabilities, which were calculated with GAMESS v. 11 [10] and AIMAll program,[11] respectively. Lowest sum of squared absolute error fitting calculations were performed with MATLAB.

[8] J. R. Alvarez-Idaboy, A. Galano, *Theor. Chem. Acc.* 2010, **126**, 75.
[9] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
[10] "General Atomic and Molecular Electronic Structure System" M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. J. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. Su, T. L. Windus, M. Dupuis, J. A. Montgomery, *J. Comput. Chem.* 1993, **14**, 1347.
[11] AIMAll (Version 13.05.06), T. A. Keith, TK Gristmill Software, Overland Park KS, USA, 2013 (aim.tkgristmill.com).

2. Tables

Table S1. Interaction energies of $C_6H_4X_2$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_6H_4X_2$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
CH_2OH	-31.6	2.30	-16.9	61.8	-93.7	-54.3
NHOH	-30.0	2.35	-12.5	55.6	-65.4	-44.8
$N(CH_3)_2$	-38.0	2.30	-16.6	90.2	-94.3	-79.3
$NHCH_3$	-37.3	2.30	-15.5	70.0	-86.6	-61.5
OCH_3	-28.8	2.30	-10.2	62.6	-57.1	-55.0
OH	-25.5	2.35	-9.0	42.2	-47.9	-34.1
CH_3	-28.9	2.30	-8.0	57.3	-45.5	-50.4
NH_2	-35.6	2.30	-14.3	50.8	-81.3	-44.7
SCH_3	-29.2	2.30	-11.9	80.4	-66.4	-70.7
SH	-24.9	2.35	-7.6	64.7	-40.3	-50.8
CCH	-24.3	2.35	-13.8	55.2	-73.5	-44.5
SiH_3	-25.1	2.35	-5.8	80.8	-30.9	-65.2
F	-16.3	2.45	-2.2	37.6	-10.3	-25.7
$COOCH_3$	-21.1	2.35	-7.3	72.8	-38.5	-58.7
COOH	-17.2	2.40	-4.3	53.6	-21.5	-39.7
$COCH_3$	-17.9	2.35	2.7	67.9	14.4	-54.7
OCF_3	-14.7	2.45	0.1	64.4	0.4	-44.0
BF_2	-14.2	2.40	7.4	50.9	37.0	-37.7
CHO	-13.5	2.40	4.5	48.6	22.2	-36.0
CF_3	-13.1	2.50	0.4	60.1	1.8	-37.9
NO	-9.3	2.50	6.9	45.8	30.2	-28.9
SiF_3	-11.9	2.45	2.3	67.0	10.8	-45.7
CN	-7.0	2.50	11.2	49.0	49.6	-30.9
NO_2	-2.6	2.60	14.0	48.3	55.1	-26.0
Cl	-18.1	2.40	-4.1	49.6	-20.5	-36.8
Br	-20.1	2.40	-5.2	60.3	-25.9	-44.7
NC	-9.8	2.45	9.1	52.9	42.8	-36.1

Table S2. Interaction energies of $C_6H_3X_3$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_6H_3X_3$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
CH_2OH	-34.2	2.30	-19.7	72.9	-111.9	-64.1
NHOH	-32.6	2.30	-15.9	64.0	-90.3	-56.3
$N(CH_3)_2$	-45.4	2.25	-21.0	113.0	-127.5	-108.5
$NHCH_3$	-44.1	2.30	-20.7	85.8	-117.6	-75.4
OCH_3	-31.1	2.30	-12.6	74.5	-71.6	-65.5
OH	-25.9	2.35	-9.9	44.7	-52.7	-36.0
CH_3	-30.2	2.30	-7.6	66.4	-43.2	-58.3
NH_2	-41.7	2.30	-18.9	57.6	-107.4	-50.6
SCH_3	-31.8	2.30	-15.6	100.1	-88.6	-88.0
SH	-24.7	2.35	-9.7	76.4	-51.8	-61.6
CCH	-23.7	2.35	-17.0	63.5	-90.6	-51.2
SiH_3	-24.6	2.30	-4.6	101.1	-26.1	-88.9
F	-11.9	2.50	0.6	37.5	2.7	-23.6
$COOCH_3$	-19.1	2.40	-8.4	89.6	-42.0	-66.4
COOH	-13.7	2.45	-3.0	61.1	-14.1	-41.7
$COCH_3$	-14.4	2.40	7.4	82.0	37.0	-60.8
OCF_3	-10.7	2.50	3.5	77.4	15.5	-48.7
BF_2	-8.5	2.45	15.0	56.7	70.5	-38.7
CHO	-8.0	2.45	11.4	53.6	53.6	-36.6
CF_3	-7.7	2.60	4.1	70.7	16.1	-38.1
NO	-2.4	2.60	14.0	49.7	55.1	-26.8
SiF_3	-6.7	2.55	6.4	81.0	26.7	-47.1
CN	0.9	2.60	19.8	54.5	77.9	-29.3
NO_2	6.5	2.75	23.8	53.9	79.1	-23.2
Cl	-15.1	2.40	-3.3	55.5	-16.3	-41.1
Br	-18.4	2.40	-4.1	71.1	-20.4	-52.7
NC	-3.4	2.55	16.7	60.2	69.5	-35.0

Table S3. Interaction energies of $C_6H_2X_4$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_6H_2X_4$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
OH	-25.1	2.35	-10.0	45.6	-53.3	-36.8
CH_3	-31.8	2.30	-7.2	73.6	-40.9	-64.7
NH_2	-35.2	2.30	-15.2	62.3	-86.4	-54.8
SH	-24.3	2.35	-6.9	88.0	-36.9	-71.0
CCH	-24.1	2.35	-21.4	71.7	-114.4	-57.8
F	-7.7	2.55	3.7	37.1	15.4	-21.6
NO	-1.0	2.55	14.9	53.7	62.0	-31.3
CN	6.5	2.75	26.0	60.0	86.4	-25.8
Cl	-13.1	2.45	-2.1	61.0	-9.7	-41.7
Br	-16.6	2.45	-3.0	81.0	-14.1	-55.3
NC	1.7	2.60	22.2	67.3	87.4	-36.2

Table S4. Interaction energies of C_6X_6 with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of C_6X_6, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
OH	-24.4	2.35	-10.7	48.6	-57.0	-39.2
CH_3	-34.4	2.25	-6.3	90.4	-38.2	-86.8
NH_2	-36.1	2.30	-13.3	73.5	-75.6	-64.6
SH	-23.3	2.35	-8.5	111.6	-45.5	-90.1
CCH	-24.9	2.40	-30.6	87.8	-153.0	-65.1
F	-0.1	2.70	9.1	36.9	32.0	-17.1
NO	9.0	3.10	24.3	61.5	56.4	-16.4
CN[a]	-	-	37.1	71.0	-	-
Cl	-10.3	2.50	-1.3	73.0	-5.9	-46.0
Br	-17.4	2.45	-6.1	100.2	-28.7	-68.4
NC	9.8	3.00	32.2	81.8	82.5	-24.8

[a] No minimum energy structure was found during the scanning (see main text).

Table S5. Interaction energies of $C_4H_2N_2X_2$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_4H_2N_2X_2$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
H	-12.1	2.50	-2.3	32.1	-10.1	-20.2
CH_2OH	-8.9	2.50	7.4	55.4	23.5	-36.0
NHOH	-19.1	2.40	-11.9	49.4	-59.3	-36.7
$N(CH_3)_2$	-26.7	2.35	-11.6	83.3	-61.9	-67.2
$NHCH_3$	-25.5	2.35	-11.6	63.6	-61.9	-51.3
OCH_3	-16.1	2.40	-5.2	55.3	-26.2	-41.0
OH	-12.2	2.50	-3.3	36.1	-14.5	-22.7
CH_3	-16.3	2.40	-2.6	51.3	-12.8	-38.0
NH_2	-23.5	2.40	-9.3	44.2	-46.4	-32.8
SCH_3	-17.8	2.40	-7.6	73.8	-38.0	-54.8
SH	-13.8	2.45	-5.6	57.2	-26.3	-39.1
CCH	-13.6	2.45	-10.2	49.0	-47.9	-33.4
SiH_3	-13.9	2.45	-1.6	74.1	-7.6	-50.6
F	-3.1	2.65	3.6	31.6	13.5	-15.8
$COOCH_3$	-9.7	2.55	-4.2	67.6	-17.5	-39.3
COOH	3.8	2.75	16.6	47.9	55.3	-20.6
$COCH_3$	-6.3	2.55	6.9	62.2	28.9	-36.2
OCF_3	-3.5	2.65	4.6	58.9	17.1	-29.4
BF_2	-3.0	2.60	11.5	45.3	45.2	-24.4
CHO	-2.5	2.60	9.2	43.2	36.3	-23.3
CF_3	-1.3	2.70	5.2	55.1	18.1	-25.5
NO	1.3	2.70	6.0	40.6	21.2	-18.8
SiF_3	-1.2	2.65	5.8	62.4	21.5	-31.1
CN	3.5	2.80	15.0	43.6	47.3	-17.5
NO_2[a]	-	-	18.2	43.4	-	-
Cl	-6.0	2.60	1.2	43.7	4.6	-23.5
Br	-8.6	2.60	-0.1	54.4	-0.5	-29.3
NC	1.1	2.70	13.1	47.2	46.1	-21.9

[a] No minimum energy structure was found during the scanning (see main text).

Table S6. Interaction energies of $C_4N_2X_4$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_4N_2X_4$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
OH	-12.6	2.45	-4.6	40.0	-21.7	-27.3
CH_3	-19.9	2.35	-2.6	68.7	-12.9	-55.4
NH_2	-23.6	2.35	-10.4	56.8	-55.6	-45.8
SH	-16.5	2.40	-10.2	81.3	-51.2	-60.3
CCH	-15.8	2.50	-19.8	65.7	-87.6	-41.4
F	4.2	3.00	9.0	31.7	23.1	-9.6
NO[a]	-	-	18.3	53.7	-	-
CN	14.1	2.85	27.8	55.4	84.3	-20.7
Cl	-2.9	2.65	2.2	55.6	8.1	-27.7
Br	-8.5	2.60	-0.9	75.7	-3.6	-40.7
NC	10.1	2.70	24.3	62.5	85.2	-28.9

[a] No minimum energy structure was found during the scanning (see main text).

Table S7. Interaction energies of $C_3N_3X_3$ with Na^+ (E_{int} in kcal mol^{-1}), equilibrium distances (R_e in Å), Θ_{zz} (in B) and α_{zz} (in a.u.) of $C_3N_3X_3$, electrostatic and polarization contributions (E_e and E_p, respectively, in kcal mol^{-1}) at the M06-2X/6-31+G* level of theory.

X	E_{int}	R_e	Θ_{zz}	α_{zz}	E_e	E_p
H	-5.5	2.65	0.9	29.1	3.3	-14.5
CH_2OH	0.4	2.65	13.5	64.5	50.3	-32.2
NHOH	-18.7	2.45	-10.4	55.0	-56.8	-37.5
$N(CH_3)_2$	-31.2	2.30	-14.0	101.3	-79.4	-89.0
$NHCH_3$	-28.6	2.30	-16.2	72.8	-91.8	-64.0
OCH_3	-13.8	2.45	-5.6	64.1	-26.1	-43.8
OH	-7.2	2.60	-2.0	35.9	-7.8	-19.3
CH_3	-11.9	2.45	-0.5	58.5	-3.1	-39.9
NH_2	-21.8	2.35	-15.7	46.8	-83.4	-37.7
SCH_3	-17.9	2.40	-9.6	91.6	-48.1	-67.9
SH	-21.1	2.50	-6.8	66.7	-14.9	-42.0
CCH	-11.4	2.60	-14.3	54.7	-56.3	-29.4
SiH_3	-11.1	2.50	-0.4	92.5	-1.9	-58.2
F[a]	-	-	8.7	29.4	-	-
$COOCH_3$	-6.5	2.70	-6.0	86.0	-21.1	-39.8
COOH	-0.1	2.90	0.7	54.5	2.1	-19.0
$COCH_3$	0.0	2.65	11.9	75.0	44.1	-37.4
OCF_3	3.0	3.05	8.1	70.2	19.8	-19.9
BF_2	4.9	2.75	19.1	49.7	63.5	-21.4
CHO	4.9	2.95	15.1	46.9	40.7	-15.2
CF_3[a]	-	-	9.6	64.8	-	-
NO[a]	-	-	15.1	46.7	-	-
SiF_3[a]	-	-	9.3	75.5	-	-
CN[a]	-	-	23.0	47.8	-	-
NO_2[a]	-	-	27.7	47.7	-	-
Cl	-0.1	2.75	3.5	47.6	11.5	-20.5
Br	-5.2	2.70	1.1	63.1	3.8	-29.2
NC[a]	-	-	19.6	53.1	-	-

[a] No minimum energy structure was found during the scanning (see main text).

3. Figures

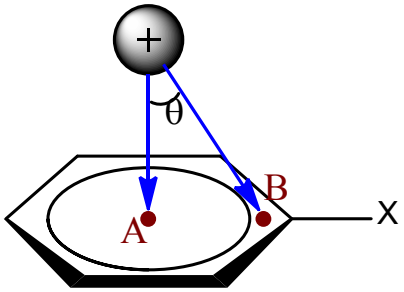

Figure S1. Graphical representation of the θ angle formed between the vectors Na^+–center of mass of the molecule (B) and Na^+–center of mass of the ring (A).

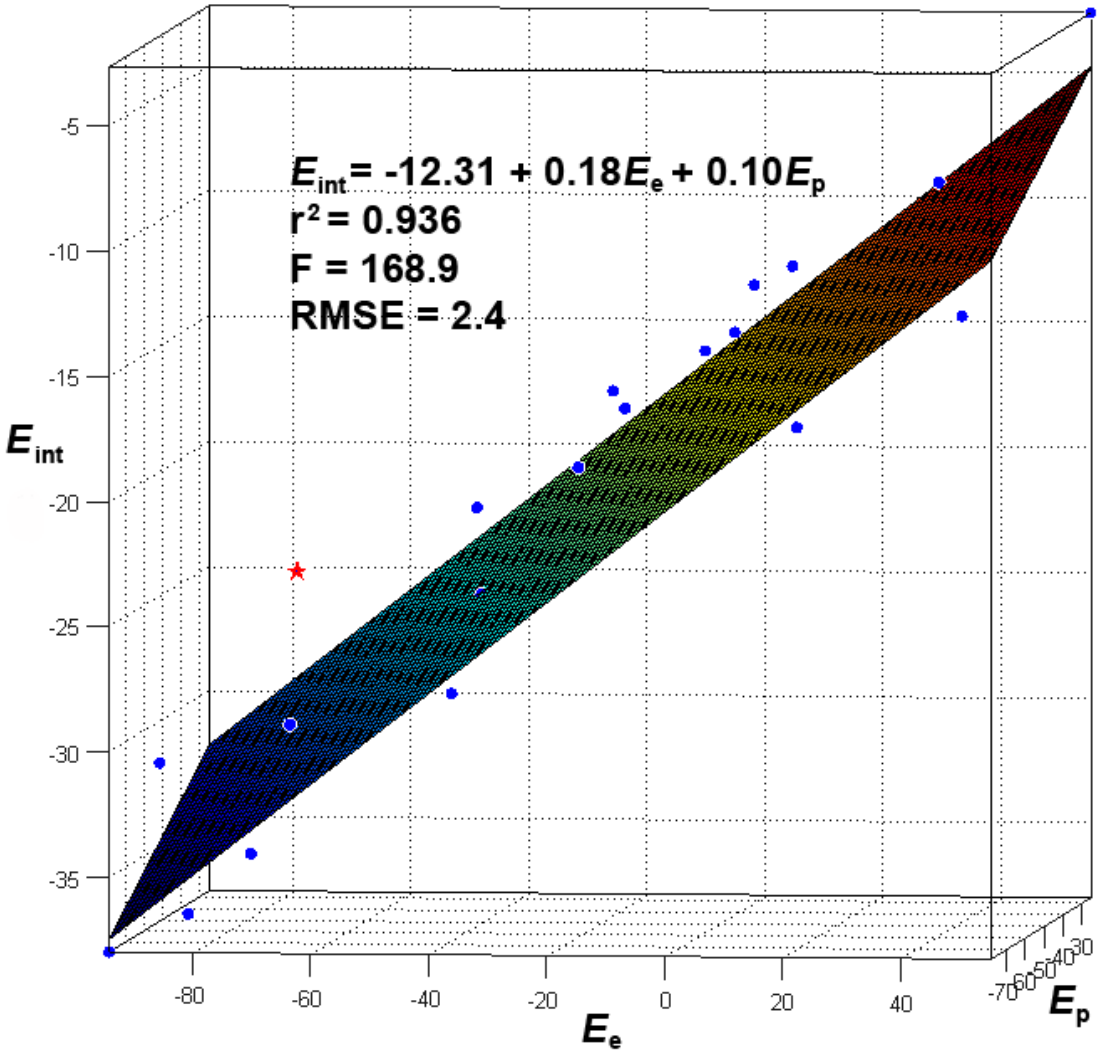

Figure S2. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_6H_4X_2$. The star represents X=CCH.

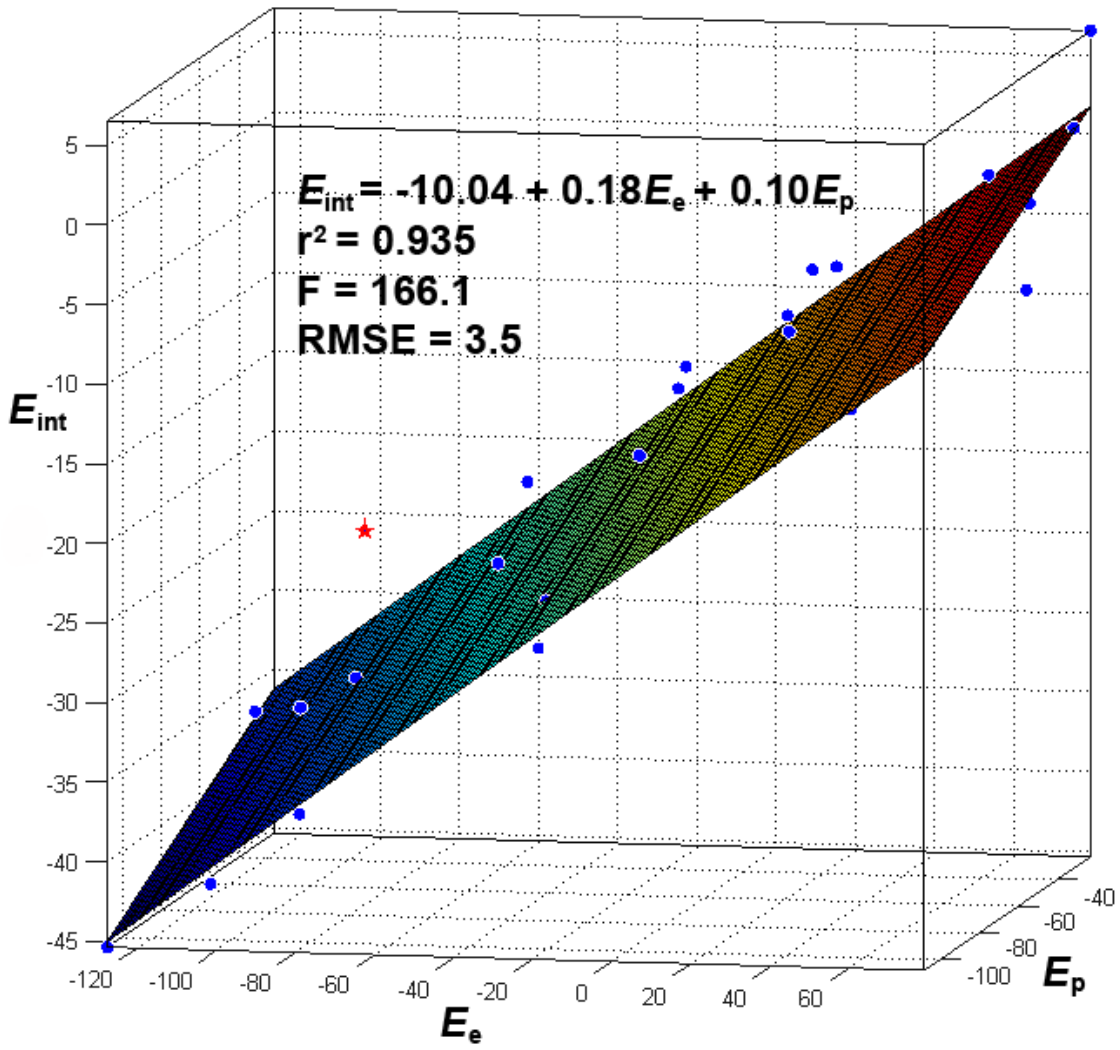

Figure S3. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_6H_3X_3$. The star represents X=CCH.

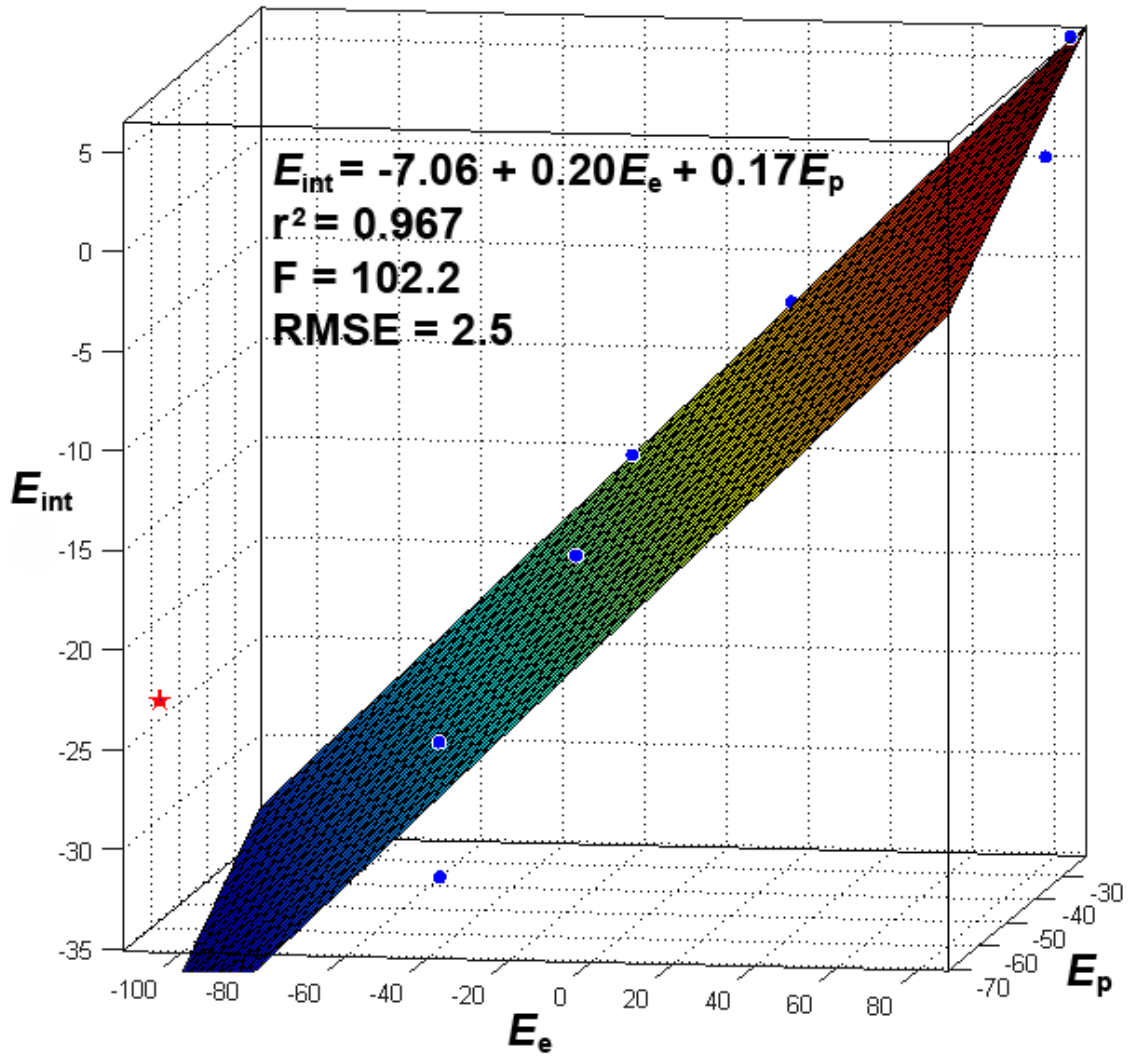

Figure S4. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_6H_2X_4$. The star represents X=CCH.

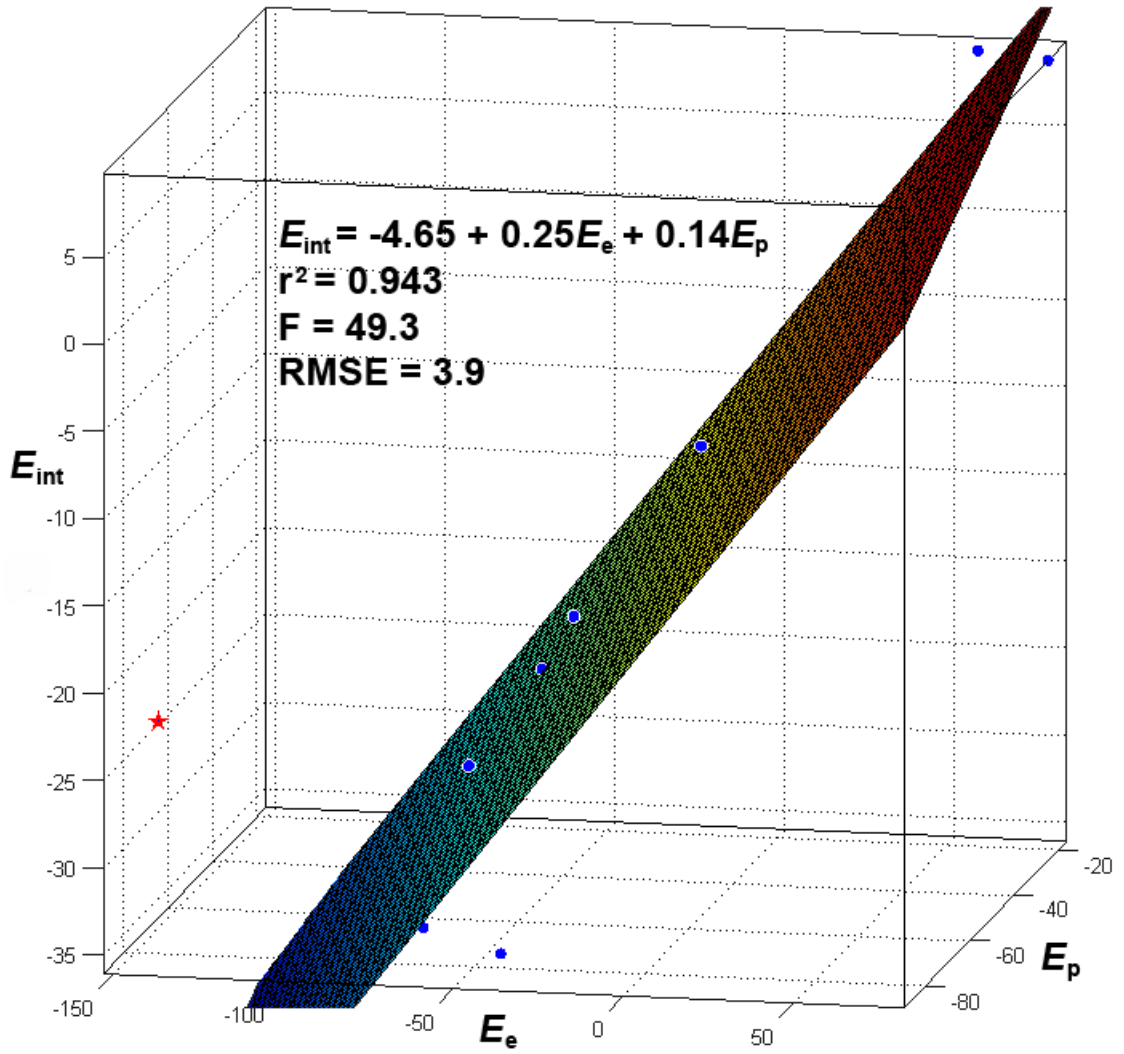

Figure S5. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for C_6X_6. The star represents X=CCH.

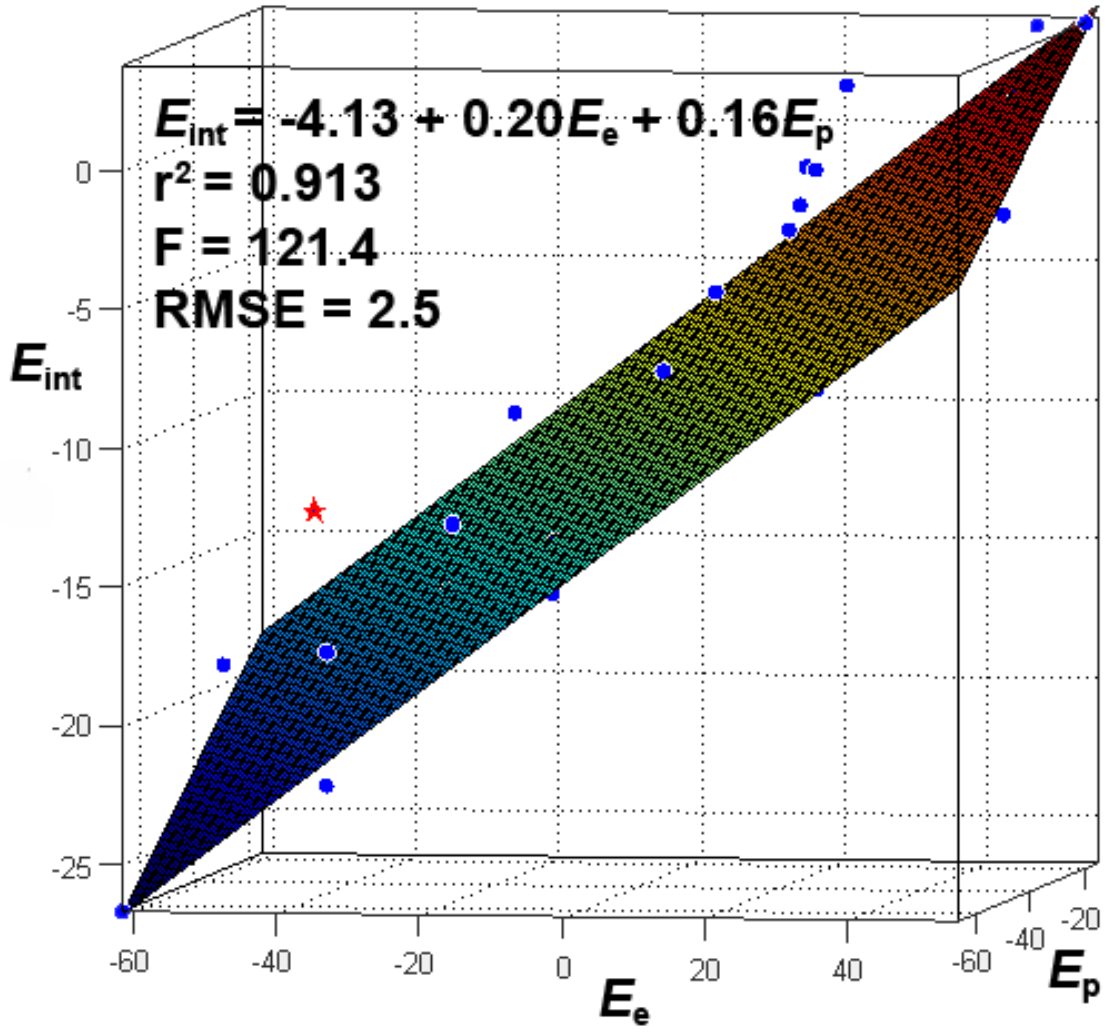

Figure S6. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_4H_2N_2X_2$. The star represents X=CCH.

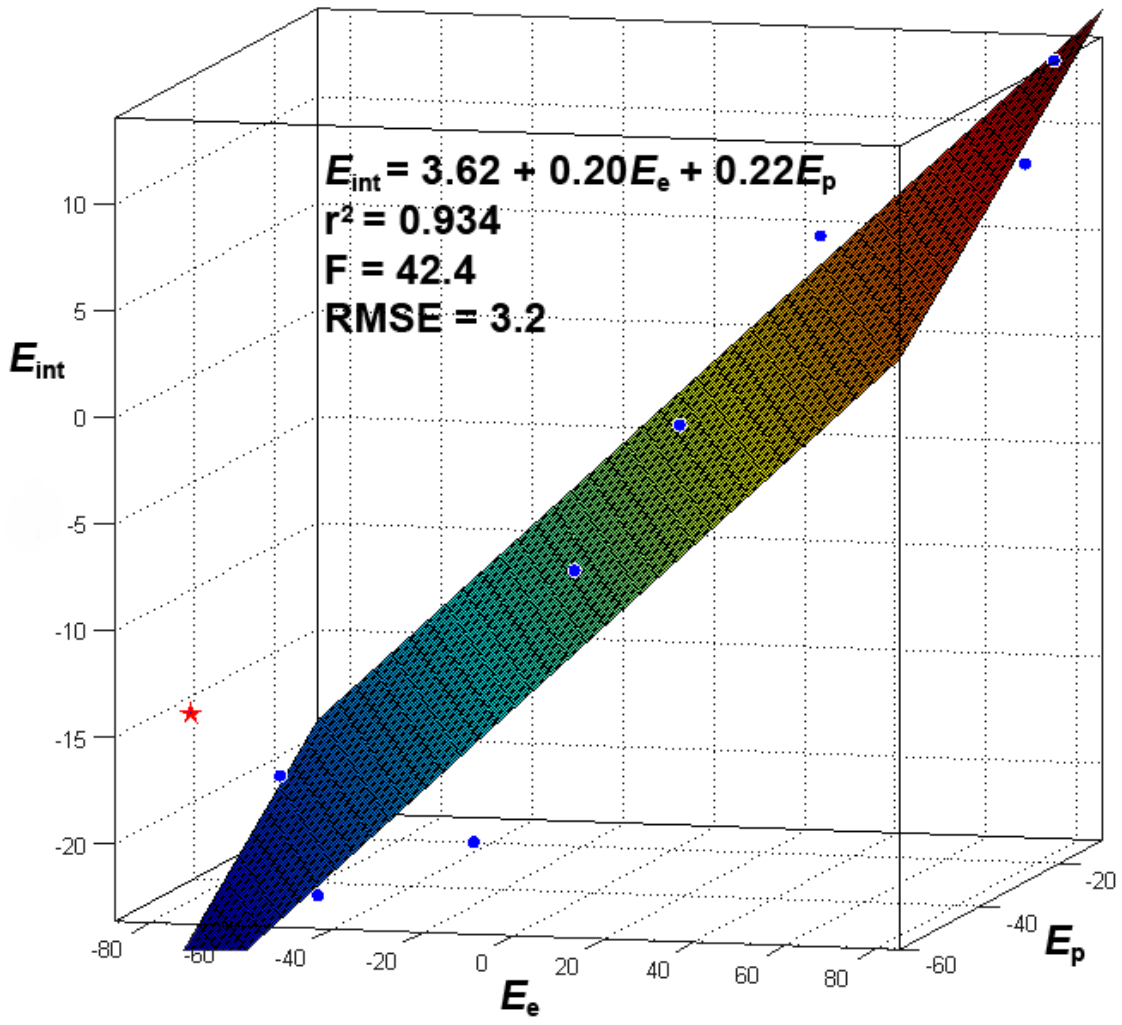

Figure S7. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_4N_2X_4$. The star represents X=CCH.

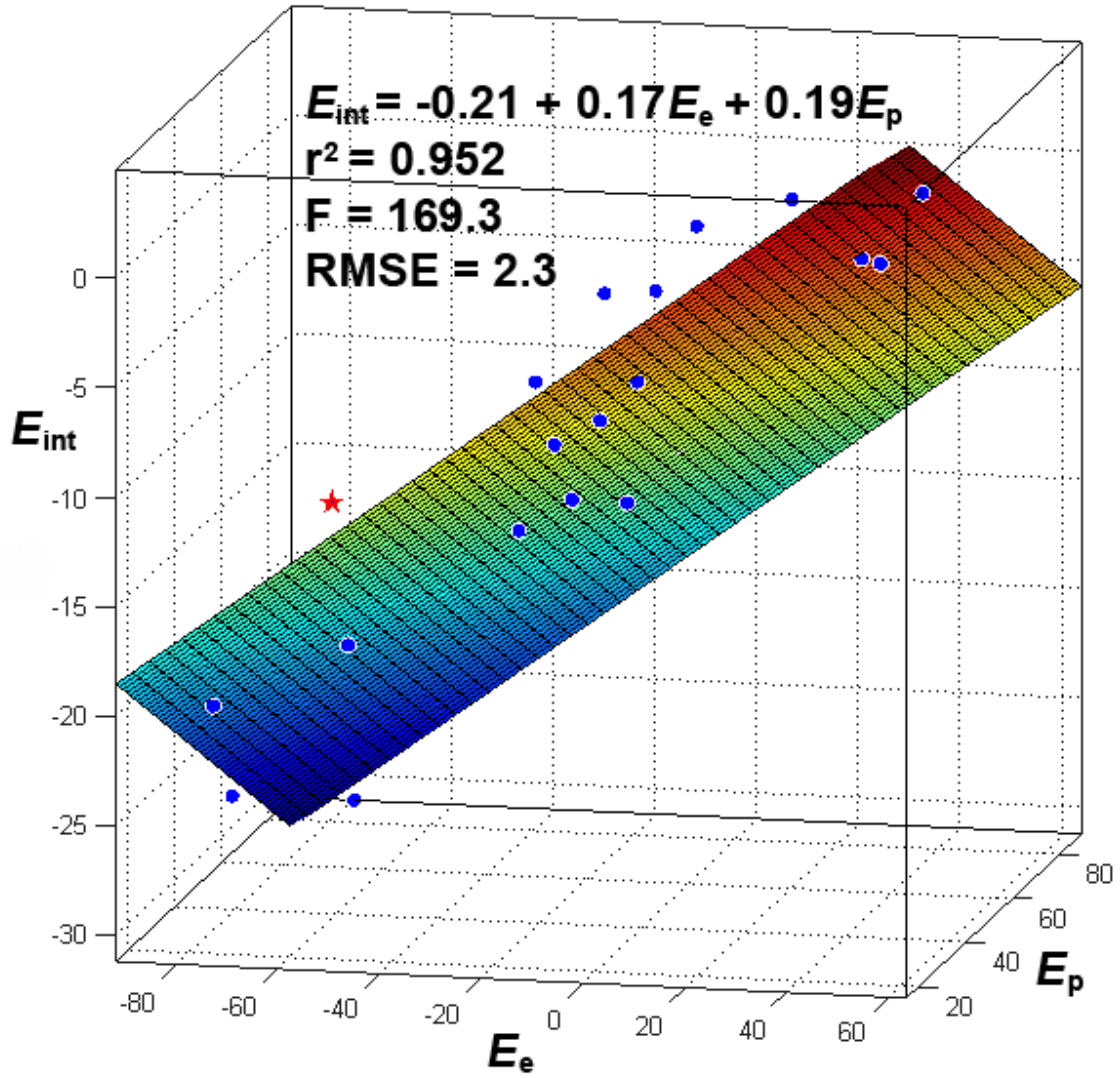

Figure S8. Interaction energy, E_{int}, plotted versus a linear combination of electrostatic, E_e, and polarization, E_p, energies (in kcal mol^{-1}) for $C_3N_3X_3$. The star represents X=CCH.

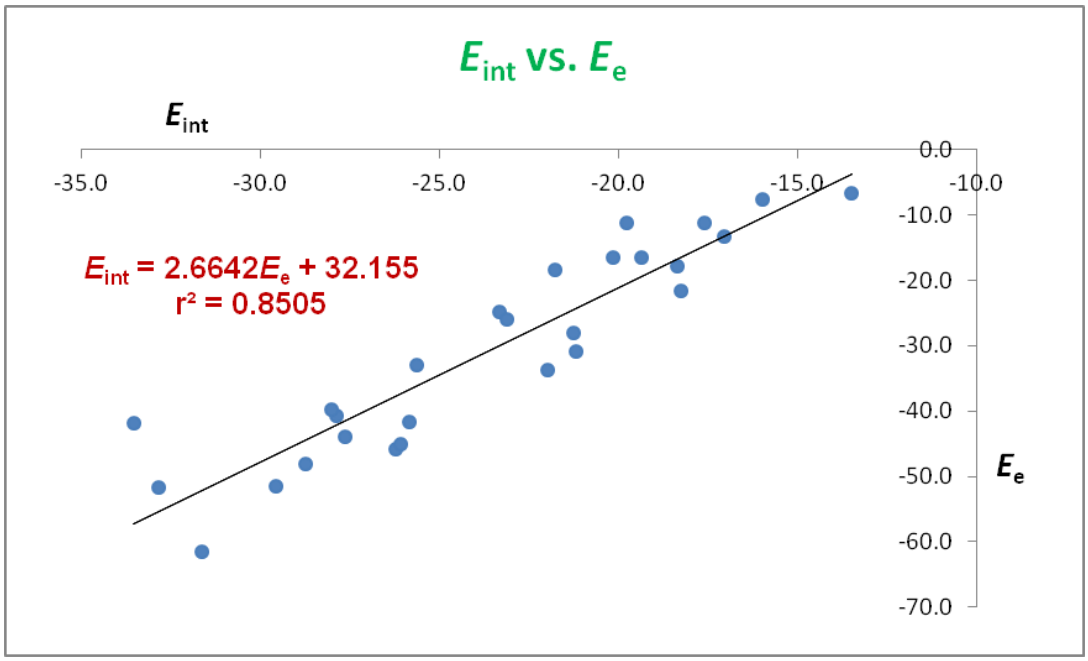

Figure S9. Interaction energy, E_{int}, plotted versus the electrostatic energy, E_e, for C_6H_5X without ethynyl group. Energies in kcal mol^{-1}.

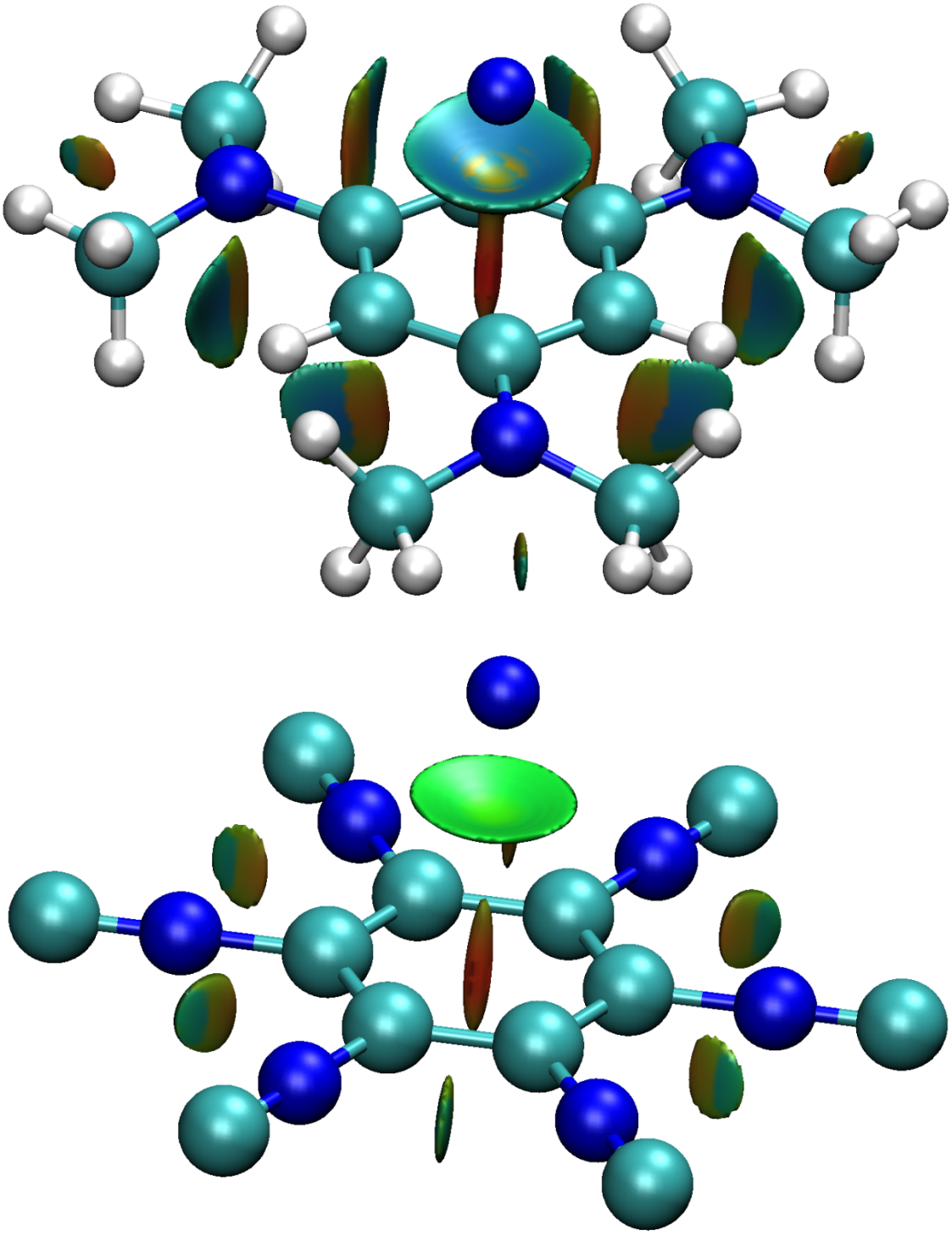

Figure S10. Tilted views of the NCIPLOT gradient isosurfaces for $C_6H_3(N(CH_3)_2)_3 \cdot Na^+$ (top) and $C_6(NC)_6 \cdot Na^+$ (bottom) complexes. Blue, green and red indicate strong attractive, weak and strong repulsive interactions, respectively.

4. Coordinates of all Na^+ Complexes

$C_6H_5X\cdots Na^+$ geometries

$C_6H_6\cdots Na^+$

C	0.00000000	1.39379772	0.00000000
C	-1.20706423	0.69689886	0.00000000
C	1.20706423	0.69689886	0.00000000
C	0.00000000	-1.39379772	0.00000000
C	1.20706423	-0.69689886	0.00000000
C	-1.20706423	-0.69689886	0.00000000
H	0.00000000	2.47706222	0.00000000
H	-2.14519881	1.23853111	0.00000000
H	-2.14519881	-1.23853111	0.00000000
H	0.00000000	-2.47706222	0.00000000
H	2.14519881	-1.23853111	0.00000000
H	2.14519881	1.23853111	0.00000000
Na	0.00000000	0.00000000	2.35000000

$C_6H_5CH_2OH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39229937
C	1.21366044	0.00000000	-0.68884432
C	2.41698814	-0.00485510	1.41416714
C	2.41346843	-0.00064321	0.01641152
C	1.20336137	-0.00258901	2.09969074
H	1.22504614	0.00458812	-1.77522581
H	-0.94127987	0.00274846	1.93494057
C	3.73558680	-0.02834005	2.14920156
H	4.24012078	-0.98631562	1.95323981
H	4.37977140	0.77443521	1.76179333
H	3.35875416	0.00342950	-0.52413279
H	1.20913341	0.00031389	3.18455021
H	-0.93786500	0.00231314	-0.54790971
O	3.50784723	0.13758066	3.53594621
H	4.35003072	0.07434246	4.00432878
Na	1.18917697	2.29844670	0.71831023

$C_6H_5NHOH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39527545
C	1.21558339	0.00000000	-0.67712189
C	2.41471725	0.00215107	1.41113246
C	2.42460593	0.00037225	0.01725813
C	1.19679150	0.00313258	2.10014454
N	3.60481666	0.07380139	2.17468548
O	4.73781998	-0.32281513	1.43915864
H	-0.93378830	-0.00197000	-0.54764469
H	-0.93688252	-0.00078103	1.93916728
H	1.23109975	-0.00560059	-1.76042882
H	3.36714480	-0.01650931	-0.51027229
H	1.19284107	0.01776720	3.18477276
H	3.55946892	-0.55056106	2.97140939
H	5.30940117	0.45496011	1.45797828
Na	1.20682255	2.30094183	0.70778156

$C_6H_5N(CH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40928297
C	1.25005770	0.00000000	-0.65071825
C	2.42354114	-0.04439491	1.47066236
C	2.43371535	-0.02727177	0.07858376
C	1.19344183	-0.02727177	2.12246141
H	-0.93012828	0.01843546	1.95826296
H	1.15368463	-0.03027988	3.20539285
H	3.37593638	-0.03027988	-0.45671118
H	1.30753744	0.01843546	-1.72924212
N	-1.18773704	-0.00986467	-0.72074706
C	-1.13064204	0.32493682	-2.13061523
H	-2.13964168	0.30136185	-2.53727291
H	-0.53977951	-0.41147366	-2.67705678
H	-0.70133649	1.32008710	-2.30981848
C	-2.41195094	0.32493682	-0.01911438
H	-2.62383062	-0.41147366	0.75730297
H	-3.23855573	0.30136185	-0.72634509
H	-2.37268092	1.32008710	0.44443166
H	3.34863201	-0.06274009	2.03202949
Na	1.18025453	-2.31563679	0.71091837

$C_6H_5NHCH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40192713
C	1.23579384	0.00000000	-0.67060150
C	2.42542563	-0.00864673	1.43612002
C	2.42675446	-0.00247455	0.03951098
C	1.20530273	-0.00842902	2.10290068
H	1.24923970	-0.00800157	-1.75540608
H	3.36530031	-0.00153916	-0.50194123
H	1.18093389	-0.01092339	3.18622083
H	-0.93302431	0.00331195	1.94918689
N	-1.17696226	-0.03217679	-0.73539534
H	-1.08089231	0.30772863	-1.67826324
C	-2.44642814	0.26452374	-0.10516355
H	-3.21651192	0.29286196	-0.87419591
H	-2.71109466	-0.52480033	0.60073452
H	-2.44213466	1.22291474	0.42911579
H	3.35636524	-0.01197373	1.98808407
Na	1.21015289	-2.30278776	0.70321598

$C_6H_5OCH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39505106
C	1.21087040	0.00000000	-0.70057942
C	2.42563477	0.00000000	1.38997597
C	2.41178674	0.00000000	-0.00740790
C	1.21910215	0.00000000	2.07798537
H	-0.92355526	0.00000000	1.95651955
H	1.21237818	0.00000000	3.16127236
H	3.34390239	0.00000000	-0.55922484
H	1.17898695	0.00000000	-1.78254801
O	-1.12634648	0.00000000	-0.76671537
C	-2.37614349	0.00000000	-0.10044819
H	-2.48965851	0.89395800	0.51798649
H	-2.48965851	-0.89395800	0.51798648

H	-3.13034139	0.00000000	-0.88253465
H	3.36419275	0.00000000	1.92914403
Na	1.21123248	2.35000000	0.69250427

$C_6H_5OH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39403795
C	1.20201229	0.00000000	-0.70504400
C	2.42133161	0.00000000	1.38427229
C	2.40853955	0.00000000	-0.00747213
C	1.21027586	0.00000000	2.07751131
H	1.19652995	0.00000000	-1.79027762
H	3.33978014	0.00000000	-0.56076937
H	1.20695847	0.00000000	3.16073093
H	-0.94806227	0.00000000	1.91615266
O	-1.21514374	0.00000000	-0.62556463
H	-1.09200212	0.00000000	-1.58256914
H	3.36029380	0.00000000	1.92259172
Na	1.20702671	2.35000000	0.69055098

$C_6H_5CH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39312582
C	1.21308388	0.00000000	-0.68500306
C	2.42757697	0.00475345	1.41706894
C	2.41457008	0.00078237	0.02002492
C	1.20468430	0.00078277	2.09267274
C	3.73013301	0.03950195	2.17742298
H	-0.93541414	-0.00457264	-0.54603795
H	-0.93746206	-0.00505267	1.93626362
H	1.22507734	-0.00505207	-1.76837205
H	3.35545447	-0.00286045	-0.51996713
H	1.19711424	-0.00286078	3.17747655
H	4.52550182	-0.45516038	1.61768699
H	4.04371128	1.07090946	2.36046998
H	3.63382028	-0.45516064	3.14522310
Na	1.20798334	2.30105270	0.70631535

$C_6H_5NH_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40045814
C	1.22749224	0.00000000	-0.67420013
C	2.42071867	-0.00762278	1.43224232
C	2.42150537	-0.00473026	0.03856701
C	1.19955026	-0.00473026	2.10386664
N	-1.20098290	0.05907406	-0.71057350
H	-0.94408616	0.01012882	1.93398409
H	1.24062791	0.01012882	-1.75853221
H	3.35210980	-0.01298687	1.98330916
H	3.35999553	-0.00784445	-0.50266426
H	1.17696694	-0.00784445	3.18700332
H	-1.15533243	-0.29633878	-1.65317580
H	-2.00519076	-0.29633878	-0.21677925
Na	1.21695038	2.29714619	0.71682254

$C_6H_5SCH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39612819
C	1.22315192	0.00000000	-0.68404754
C	2.42165842	0.00000000	1.41398150
C	2.42071218	0.00000000	0.01844258
C	1.20874084	0.00000000	2.09332469
H	-0.92757507	0.00000000	1.95205704
H	1.19291823	0.00000000	3.17669038
H	3.35715861	0.00000000	-0.52618989
H	1.22925374	0.00000000	-1.76823713
S	-1.46082663	0.00000000	-1.00205444
C	-2.78656822	0.00000000	0.22815778
H	-2.75369640	0.89486399	0.84906533
H	-2.75369640	-0.89486400	0.84906532
H	-3.71588025	0.00000000	-0.33997300
H	3.35598055	0.00000000	1.96101757
Na	1.21237731	2.30000000	0.70630475

$C_6H_5SH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39782446
C	1.21525441	0.00000000	-0.68989256
C	2.41830014	-0.00806424	1.40899179
C	2.41630075	-0.01297569	0.01538745
C	1.20526548	0.00186170	2.09519073
H	1.22670135	0.01333692	-1.77657706
H	3.35500527	-0.01939061	-0.53128453
H	1.19307255	0.00193069	3.18132563
H	-0.94281177	-0.01106372	1.93814404
S	-1.57229638	0.04204668	-0.82966003
H	-1.12076715	-0.35773384	-2.02802273
H	3.35654972	-0.01337389	1.95498656
Na	1.23295641	2.34694009	0.68958656

$C_6H_5CCH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40106999
C	1.21868336	0.00000000	-0.69123655
C	2.41397797	0.00000000	1.40604387
C	2.41814303	0.00000000	0.01204975
C	1.20350424	0.00000000	2.09741232
C	-1.24037794	-0.00000000	-0.72246964
C	-2.28400687	-0.00000000	-1.33034100
H	-0.94442794	0.00000000	1.92994106
H	1.21276165	0.00000000	-1.77364761
H	3.34989306	0.00000000	1.95117630
H	3.35681725	0.00000000	-0.52809758
H	1.19677894	0.00000000	3.18038194
H	-3.20487290	-0.00000000	-1.86670797
Na	1.20905151	2.35000000	0.70422327

$C_6H_5SiH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40111300
C	1.23426792	0.00000000	-0.66316501
C	2.41206141	0.01491037	1.44218554
C	2.43161187	0.00935963	0.04907365
C	1.19415795	0.00934169	2.11875918

Si	-1.61036329	0.01945329	-0.96288305
H	-0.94052387	-0.01167151	1.94176968
H	1.26542009	-0.01167474	-1.74757788
H	3.34172171	0.01962886	1.99802473
H	3.37629991	0.00824453	-0.48101089
H	1.17432473	0.00819840	3.20182466
H	-2.06136347	1.41150972	-1.24149735
H	-2.67232185	-0.66312975	-0.17423315
H	-1.42288163	-0.67640615	-2.26530910
Na	1.20115495	2.35557663	0.72466122

$C_6H_5F\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38479524
C	1.16230278	0.00000000	-0.75280150
C	2.41878668	0.00000000	1.31519778
C	2.38146717	0.00000000	-0.07835787
C	1.22884340	0.00000000	2.04143816
F	-1.18927879	0.00000000	-0.64666175
H	-0.93990257	0.00000000	1.92027724
H	1.10080066	0.00000000	-1.83279007
H	3.36951520	0.00000000	1.83214955
H	3.30373749	-0.00000000	-0.64562581
H	1.25408133	-0.00000000	3.12390686
Na	1.19856676	2.35000000	0.65171202

$C_6H_5COOCH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39607692
C	1.20514051	0.00000000	-0.70533081
C	2.41091926	0.00000000	1.38527385
C	2.40989802	0.00000000	-0.00865851
C	1.20607792	0.00000000	2.08760133
C	-1.31835096	0.00000000	-0.69154025
O	-2.38783740	0.00000000	-0.12310079
O	-1.20504131	-0.00000000	-2.03007569
C	-2.44986855	-0.00000000	-2.74287365
H	-0.94867696	0.00000000	1.91710425
H	1.19313778	0.00000000	-1.78664201
H	3.35047366	0.00000000	1.92437238
H	3.34638320	0.00000000	-0.55239782
H	1.20824866	0.00000000	3.17044408
H	-2.18016449	-0.00000000	-3.79443760
H	-3.02462981	-0.88838823	-2.48793554
H	-3.02462880	0.88838940	-2.48793542
Na	1.20533928	2.35000000	0.69249420

$C_6H_5COOH\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39392799
C	1.20439882	0.00000000	-0.70355192
C	2.40873353	0.00000000	1.38334304
C	2.41050294	0.00000000	-0.01284688
C	1.20465678	0.00000000	2.09045789
C	3.72090572	0.00000000	2.07724866
O	4.79691825	0.00000000	1.52409387
O	3.61163590	0.00000000	3.42322485
H	-0.93931672	0.00000000	-0.53898926
H	-0.93640704	-0.00000000	1.93710783
H	1.20137767	-0.00000000	-1.78606346
H	3.35920556	0.00000000	-0.53337130
H	1.21745046	-0.00000000	3.17168389
H	4.51621829	0.00000000	3.77482328
Na	1.20471522	2.35000000	0.69188867

$C_6H_5COCH_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39855087
C	1.21525452	0.00000000	-0.68987624
C	2.41148145	0.00000000	1.40422467
C	2.41859269	0.00000000	0.01150768
C	1.20042512	0.00000000	2.09773310
C	-1.31990788	-0.00000000	-0.70904870
O	-2.36021364	-0.00000000	-0.07881643
C	-1.33369105	-0.00000000	-2.22114071
H	-0.95185502	0.00000000	1.91348348
H	1.23240150	0.00000000	-1.77228048
H	3.34744194	-0.00000000	1.94921388
H	3.35745859	0.00000000	-0.52786872
H	1.19571482	-0.00000000	3.18055114
H	-0.82250392	-0.88309888	-2.61121925
H	-0.82250347	0.88309829	-2.61121957
H	-2.36873636	-0.00000000	-2.55474336
Na	1.20762640	2.35000000	0.70368990

$C_6H_5OCF_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38956700
C	1.18133965	0.00000000	-0.73045135
C	2.41408842	0.00000000	1.35819605
C	2.38919791	0.00000000	-0.03241098
C	1.21338213	0.00000000	2.06681309
C	-1.44876232	-0.00000000	-1.89715997
O	-1.27919212	-0.00000000	-0.56511632
F	-0.91008594	-1.08123239	-2.48971703
F	-0.91008518	1.08123336	-2.48971691
F	-2.75558696	-0.00000000	-2.14481302
H	-0.94641366	0.00000000	1.91389030
H	1.18052072	-0.00000000	-1.81001841
H	3.35893492	-0.00000000	1.88593513
H	3.31562233	0.00000000	-0.59251890
H	1.21807310	-0.00000000	3.14938729
Na	1.19966772	2.40000000	0.67528533

$C_6H_5BF_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39441352
C	1.20314406	0.00000000	-0.70486412
C	2.42515975	0.00000000	1.38991457
C	2.40922917	0.00000000	-0.01154755
C	1.20788116	0.00000000	2.08459628
F	3.80911027	0.00000000	3.49076344
F	4.93741373	0.00000000	1.52206967
B	3.76624246	0.00000000	2.15851976

H	-0.94001747	0.00000000	-0.53874553
H	-0.93697406	0.00000000	1.93731895
H	1.19794766	0.00000000	-1.78774901
H	3.34642794	-0.00000000	-0.55565659
H	1.21215265	-0.00000000	3.16828347
Na	1.20756923	2.35000000	0.69208556

$C_6H_5CHO\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39802508
C	1.20374071	0.00000000	-0.70564215
C	2.41226178	0.00000000	1.37649855
C	2.41370436	0.00000000	-0.01673192
C	1.20726920	0.00000000	2.08399294
C	-1.27860787	-0.00000000	-0.74641100
O	-2.37317065	-0.00000000	-0.22773075
H	-0.94916428	0.00000000	1.91934610
H	1.19013733	-0.00000000	-1.79064638
H	3.35200021	0.00000000	1.91526111
H	3.35013043	0.00000000	-0.56026585
H	1.21649154	0.00000000	3.16681003
H	-1.18057499	-0.00000000	-1.84674071
Na	1.20616249	2.35000000	0.68935684

$C_6H_5CF_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39337768
C	1.20472214	0.00000000	-0.70010423
C	2.40433194	0.00105775	1.38360495
C	2.41291049	-0.00009533	-0.00928729
C	1.20433982	-0.00009533	2.09088232
H	1.20516918	0.00336227	-1.78261446
H	-0.93571979	0.00336227	1.93767272
C	3.70290947	-0.05247898	2.13088874
F	4.70286212	0.54571078	1.45382567
F	4.09822648	-1.32504816	2.35837920
F	3.61994431	0.54571078	3.33564452
H	3.35318213	0.00501655	-0.54494606
H	1.21364682	0.00501655	3.17298882
H	-0.93855025	0.00261910	-0.54010128
Na	1.20573911	-2.39971182	0.69408542

$C_6H_5NO\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39240229
C	1.18914268	0.00000000	-0.73307817
C	2.40589126	0.00000000	1.35284736
C	2.39452290	0.00000000	-0.04633855
C	1.21379982	0.00000000	2.07392087
N	-1.30522174	-0.00000000	-0.60829535
O	-1.30067042	-0.00000000	-1.81397843
H	-0.94989253	-0.00000000	1.91284577
H	1.14641713	0.00000000	-1.81416724
H	3.35208720	-0.00000000	1.87965624
H	3.32915745	0.00000000	-0.59286370
H	1.23211540	-0.00000000	3.15614273
Na	1.20055918	2.40000000	0.67329230

$C_6H_5SiF_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40151428
C	1.22365603	0.00000000	-0.68330681
C	2.41063799	-0.01734446	1.41488962
C	2.42366369	-0.01045203	0.02133366
C	1.20028100	-0.01045203	2.10568904
Si	-1.57878858	-0.00699802	-0.92664746
F	-2.12660185	-1.47321382	-1.24817866
F	-2.73273374	0.71969820	-0.09474458
F	-1.41506253	0.71969820	-2.33974534
H	1.24108835	0.01565415	-1.76711757
H	-0.93777136	0.01565415	1.94514516
H	3.36474484	-0.00915219	-0.51381835
H	1.19186522	-0.00915219	3.18825570
H	3.34456535	-0.02404804	1.96304498
Na	1.17347042	-2.40546509	0.68832542

$C_6H_5CN\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39404094
C	1.20383069	0.00000000	-0.70295221
C	2.40798453	0.00000000	1.38236297
C	2.41257969	0.00000000	-0.01624897
C	1.20252365	0.00000000	2.09158831
C	3.65664020	-0.00000000	2.09918459
N	4.65934892	-0.00000000	2.67481429
H	-0.93908285	-0.00000000	-0.53910370
H	-0.93591581	0.00000000	1.93774920
H	1.20141226	0.00000000	-1.78533440
H	3.35467589	-0.00000000	-0.54844038
H	1.21800401	-0.00000000	3.17350018
Na	1.20448703	2.40000000	0.69146552

$C_6H_5NO_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38887182
C	1.16719204	0.00000000	-0.75274675
C	2.41321173	0.00000000	1.31521157
C	1.22575579	0.00000000	2.04608031
C	2.38384298	0.00000000	-0.07883226
O	-2.30214791	-0.00000000	-0.02698152
O	-1.27040304	-0.00000000	-1.92007529
N	-1.29135054	-0.00000000	-0.70379203
H	-0.93707823	-0.00000000	1.92634827
H	1.11099941	-0.00000000	-1.83156042
H	3.36375815	-0.00000000	1.83326377
H	1.25254014	0.00000000	3.12798572
H	3.30758065	0.00000000	-0.64269877
Na	1.19833366	2.45000000	0.65309740

$C_6H_5Cl\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39373223
C	1.20204805	0.00000000	2.09948774
C	2.41163099	0.00000000	1.40672554

C	2.42664877	0.00000000	0.01307423
C	1.21699442	0.00000000	-0.67464200
H	-0.92929805	0.00000000	-0.56024690
H	-0.94606507	0.00000000	1.92667586
H	1.19619954	0.00000000	3.18500298
H	3.35189855	0.00000000	1.94983230
H	3.36192966	0.00000000	-0.53712675
Cl	1.22639863	0.00000000	-2.42011567
Na	1.20955624	-2.35000000	0.70592596

$C_6H_5Br\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39338889
C	1.20022204	0.00000000	2.10121575
C	2.40812390	0.00000000	1.40657563
C	2.42338367	0.00000000	0.01327030
C	1.21543616	0.00000000	-0.67714260
H	-0.93145436	0.00000000	-0.55582084
H	-0.94667436	0.00000000	1.92484200
H	1.19427927	0.00000000	3.18646648
H	3.34892125	0.00000000	1.94836443
H	3.36086928	0.00000000	-0.53231633
Br	1.22575456	0.00000000	-2.56145735
Na	1.20785966	-2.35000000	0.70645666

$C_6H_5NC\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39133444
C	1.20371854	0.00000000	2.09522528
C	2.41552730	0.00000000	1.40535560
C	2.43167903	0.00000000	0.01411492
C	1.21981901	0.00000000	-0.67851999
H	-0.92482408	-0.00000000	-0.56723170
H	-0.94462064	0.00000000	1.92638941
H	1.19741709	0.00000000	3.18082199
H	3.35387294	0.00000000	1.95134043
H	3.36302567	0.00000000	-0.54234246
N	1.22788265	0.00000000	-2.06770059
C	1.23469705	0.00000000	-3.24166681
Na	1.21179023	-2.40000000	0.70465671

$C_6H_4X_2\cdots Na^+$ geometries

$C_6H_4(CH_2OH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39052327
C	1.22356556	0.00000000	-0.67658350
C	2.41995040	0.00000000	1.42631990
C	2.41924512	0.00000000	0.02815059
C	1.20341578	0.00000000	2.09981709
C	-1.28044105	0.00000000	-0.79782698
C	3.73812870	0.00000000	2.16012038
O	-2.39112745	0.00000000	0.08594488
O	3.50289718	0.00000000	3.55988576
H	-0.94413328	-0.00000000	1.91784978
H	1.24030609	0.00000000	-1.76221395
H	3.36092826	0.00000000	-0.51231825
H	1.19935986	-0.00000000	3.18122563
H	-1.30426017	0.88670288	-1.44111644
H	-1.30425896	-0.88670317	-1.44111703
H	4.31246295	-0.88670386	1.86938283
H	4.31246414	0.88670219	1.86938215
H	-3.20439198	0.00000000	-0.42968369
H	4.34791102	0.00000000	4.02164722
Na	1.21102962	2.30000000	0.71137098

$C_6H_4(NHOH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.77948964
C	1.19963596	0.00000000	0.69348116
C	-1.21681565	0.00097644	0.69068066
C	-1.20898436	-0.00000000	2.08060439
C	1.20837345	0.00097644	2.09262510
N	2.46792807	-0.06603193	2.74942931
N	-2.41457130	-0.06603193	-0.07302806
O	2.36680182	0.28388457	4.11147396
O	-3.54440960	0.28388457	0.69434249
H	0.00510644	-0.01660012	-1.08450541
H	0.00132619	0.01896995	3.85979888
H	2.13688662	-0.01660012	0.14782628
H	-2.14580899	0.01896995	2.61859083
H	3.10947668	0.60787674	2.34719313
H	-2.38617499	0.60787674	-0.82971308
H	2.68109661	-0.50290558	4.57390865
H	-4.10199225	-0.50290558	0.65276547
Na	-0.25913365	-2.33567092	1.38948047

$C_6H_4(NHCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39070400
C	1.19207127	0.00000000	2.13166000
C	2.38361987	0.03758095	1.39062900
C	2.38361987	0.03758095	0.00007500
C	1.19207127	0.00000000	-0.74095600
H	-0.95826439	0.00243269	-0.49959700
H	-0.95826439	0.00243269	1.89030100
H	3.34131146	0.06985368	1.89030600
H	3.34131146	0.06985368	-0.49960200
N	1.19308702	-0.04668507	-2.14231600
N	1.19308702	-0.04668507	3.53302000
C	2.40870467	0.38258580	-2.80739600
H	2.25526003	0.33107608	-3.88412399
H	3.23488139	-0.28631963	-2.56467200
H	2.69890835	1.40928541	-2.53958900
C	2.40870467	0.38258580	4.19810000
H	3.23488139	-0.28631963	3.95537600
H	2.25526003	0.33107608	5.27482799
H	2.69890835	1.40928541	3.93029300
C	-0.03831221	0.33440940	-2.80750200
H	-0.83788563	-0.36551867	-2.56306200
H	0.11656036	0.28706920	-3.88421400
H	-0.36788243	1.34962638	-2.54134300

C	-0.03831221	0.33440940	4.19820600
H	0.11656036	0.28706920	5.27491800
H	-0.83788563	-0.36551867	3.95376600
H	-0.36788243	1.34962638	3.93204700
Na	1.25424987	-2.28635190	0.67634331

$C_6H_4(NHCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40538623
C	1.23583922	0.00000000	-0.64619494
C	1.18172324	0.00307585	2.12285443
C	2.43181348	0.00311295	0.07992559
C	2.42861548	0.00632133	1.47450293
N	3.60282066	0.05403505	2.23690411
N	-1.21829038	0.04148640	-0.69017200
C	4.86714452	-0.24990076	1.59794830
C	-1.23349968	-0.26577985	-2.10598006
H	-0.94624590	0.01247709	1.93589214
H	1.28953592	-0.00370538	-1.72661655
H	1.14752366	0.01792686	3.20709764
H	3.36563189	0.00169840	-0.46614134
H	3.49588391	-0.37950018	3.14077090
H	-1.96924116	-0.39372511	-0.17731012
H	5.64326756	-0.28195118	2.36099714
H	5.12834933	0.54110037	0.89280901
H	4.85815921	-1.20643861	1.05819558
H	-0.73139182	0.52584831	-2.66485813
H	-2.26841668	-0.30254414	-2.44248109
H	-0.74683475	-1.22102760	-2.34480504
Na	1.20904533	2.30208160	0.73941208

$C_6H_4(OCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38875900
C	1.21282569	0.00000000	2.09408936
C	2.41987861	0.00000000	1.40730351
C	2.41440926	0.00000000	0.00603464
C	1.22063076	0.00000000	-0.68821864
O	3.65206534	-0.00000000	1.99809133
O	-1.12284463	-0.00000000	-0.77880315
C	3.69276465	-0.00000000	3.41198461
C	-2.37187036	-0.00000000	-0.11496177
H	-0.92328909	-0.00000000	1.95061138
H	1.18108247	0.00000000	3.17442875
H	3.36362716	-0.00000000	-0.51403767
H	1.20323781	-0.00000000	-1.77043272
H	3.21097583	0.89375766	3.81766054
H	3.21097643	-0.89375831	3.81766001
H	4.74529257	-0.00000000	3.68164804
H	-2.48620738	0.89375766	0.50440926
H	-2.48620722	-0.89375831	0.50440847
H	-3.12675966	-0.00000000	-0.89641909
Na	1.21129055	2.30000000	0.70132827

$C_6H_4(OH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.78868400
C	1.20279723	0.00000000	0.69635300
C	1.20279723	0.00000000	2.09233100
C	-1.20585324	-0.00000000	2.08798900
C	-1.20585324	-0.00000000	0.70069500
O	-0.06669407	-0.00000000	-1.36940200
O	-0.06669407	-0.00000000	4.15808600
H	2.14615420	-0.00000000	0.16050800
H	2.14615420	0.00000000	2.62817600
H	-2.13360519	-0.00000000	2.64523100
H	-2.13360519	-0.00000000	0.14345300
H	0.82327285	-0.00000000	-1.74114400
H	0.82327285	-0.00000503	4.52982800
Na	-0.00101900	-2.35000000	1.39434200

$C_6H_4(CH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39626418
C	1.23419152	0.00000000	-0.65293564
C	2.42698821	0.01562180	1.46172582
C	2.42702574	0.00767792	0.06548424
C	1.19283422	0.00767792	2.11468406
C	-1.29213981	0.02190334	-0.77822962
C	3.71884255	0.05415753	2.23978351
H	-0.94524155	-0.01190464	1.92889147
H	1.26296989	-0.01190464	-1.73753014
H	3.37235189	0.00167282	-0.46709210
H	1.16414045	0.00167282	3.19932951
H	-1.17903105	-0.47696335	-1.74223805
H	-1.61240986	1.04957051	-0.97112178
H	-2.09135697	-0.47696335	-0.22745038
H	4.02938536	1.08588506	2.42681715
H	4.52275135	-0.44026268	1.69182995
H	3.61042543	-0.44026268	3.20661762
Na	1.20372122	2.30514212	0.73087044

$C_6H_4(NH_2)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39072200
C	2.39422000	0.00000000	1.39072200
C	2.39422000	0.00000000	-0.00000000
C	1.19711000	0.00414600	-0.72036900
C	1.19711000	0.00414600	2.11109100
H	-0.94499500	-0.01110600	-0.53214800
H	-0.94499500	-0.01110600	1.92287000
H	3.33921500	-0.01110600	1.92287000
H	3.33921500	-0.01110600	-0.53214800
H	0.36803600	0.33612900	3.94029200
H	2.02618400	0.33612900	3.94029200
H	0.36803600	0.33612900	-2.54957000
H	2.02618400	0.33612900	-2.54957000
N	1.19711000	-0.05386700	3.51697800
N	1.19711000	-0.05386700	-2.12625600
Na	1.19401179	-2.29907511	0.69613093

$C_6H_4(SCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39212468

C	1.20172886	0.00000000	2.10591520
C	2.42420057	0.00000000	1.43990166
C	2.42227982	0.00000000	0.03690598
C	1.23293683	0.00000000	-0.66952771
S	4.00883128	-0.00000000	2.23116909
S	-1.45295000	-0.00000000	-1.01296343
C	3.56885237	-0.00000000	3.98538949
C	-2.78289762	-0.00000000	0.21264252
H	-0.92697702	-0.00000000	1.94944552
H	1.15580645	-0.00000000	3.18655577
H	3.36344586	0.00000000	-0.50108238
H	1.25509450	0.00000000	-1.75337918
H	3.00846524	0.89494484	4.25478994
H	3.00846516	-0.89494542	4.25479036
H	4.51358374	-0.00000000	4.52728945
H	-2.75136956	0.89494484	0.83362266
H	-2.75136990	-0.89494542	0.83362292
H	-3.71073208	-0.00000000	-0.35770486
Na	1.21352439	2.30000000	0.71755323

$C_6H_4(SH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.80685800
C	1.20464029	0.00000000	0.70814000
C	1.20464029	0.00000000	2.09871800
C	-1.20337714	-0.00945711	2.09950500
C	-1.20337714	-0.00945711	0.70735300
H	2.15157306	-0.01590622	0.17515100
H	2.15157306	-0.01590622	2.63170700
H	-2.14714507	0.00904156	2.63729200
H	-2.14714507	0.00904156	0.16956600
S	-0.06049240	-0.04686893	-1.77846600
S	-0.06049240	-0.04686893	4.58532400
H	1.08463677	0.62373152	-1.98303800
H	1.08463677	0.62373152	4.78989600
Na	0.00427829	-2.35313770	1.40208701

$C_6H_4(CCH)_2\cdots Na^+$

C	-1.40053000	0.00000000	0.00000000
C	-0.69346500	1.21011600	0.00000000
C	-0.69346500	-1.21011600	0.00000000
C	1.40053000	0.00000000	0.00000000
C	0.69346500	-1.21011600	0.00000000
C	0.69346500	1.21011600	0.00000000
H	-1.24069100	-2.14358900	0.00000000
H	-1.24069100	2.14358900	0.00000000
H	1.24069100	-2.14358900	0.00000000
H	1.24069100	2.14358900	0.00000000
C	-2.83454200	0.00000000	0.00000000
C	-4.04230000	0.00000000	0.00000000
H	-5.10788400	0.00000000	0.00000000
C	2.83454200	0.00000000	0.00000000
C	4.04230000	0.00000000	0.00000000
H	5.10788400	0.00000000	0.00000000
Na	0.00000000	0.00000000	2.35000000

$C_6H_4(SiH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40049051
C	1.23572272	0.00000000	-0.65906223
C	2.42995144	-0.01804031	1.45796034
C	2.43000152	-0.00886650	0.05749988
C	1.19427879	-0.00886650	2.11705262
Si	-1.60985649	-0.01767579	-0.96590692
Si	4.03948447	-0.05961732	2.42367319
H	-0.93977305	0.01504408	1.94282318
H	1.27199851	0.01504408	-1.74348935
H	3.36990219	-0.00053106	-0.48475622
H	1.15813064	-0.00053106	3.20155631
H	-2.06032383	-1.41116876	-1.23618538
H	-2.66924041	0.67154002	-0.18027469
H	-1.41519349	0.67154002	-2.27036796
H	4.47470189	-1.45968575	2.68480176
H	3.85231092	0.62312307	3.73262786
H	5.10635783	0.62312307	1.64253459
Na	1.22652421	2.34400949	0.72899019

$C_6H_4F_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38524842
C	1.16554233	0.00000000	-0.74861489
C	2.38799279	0.00000000	1.30435097
C	2.38799279	-0.00000000	-0.08089745
C	1.22245046	0.00000000	2.05296587
F	-1.18719312	0.00000000	-0.64845945
F	3.57518590	-0.00000000	1.95281042
H	-0.93896162	0.00000000	1.92201865
H	1.10974567	-0.00000000	-1.82873431
H	3.32695441	-0.00000000	-0.61766768
H	1.27824712	-0.00000000	3.13308528
Na	1.19399639	2.45000000	0.65217548

$C_6H_4(COOCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.77467200
C	1.21182200	0.00000000	0.69335400
C	-1.21262900	0.00000000	0.69230900
C	-1.21262900	0.00000000	2.08236300
C	1.21182200	0.00000000	2.08131800
H	-2.14400499	0.00000000	0.14313500
H	2.13635200	0.00000000	0.13097200
H	-2.14400499	0.00000000	2.63153700
H	2.13635200	0.00000000	2.64370000
C	0.05580801	0.00000000	4.26518900
C	0.05580801	0.00000000	-1.49051700
O	1.08265100	0.00000000	4.90588300
O	1.08265100	0.00000000	-2.13121100
O	-1.16060899	0.00000000	4.83066000
O	-1.16060899	0.00000000	-2.05598800
C	-1.16084300	0.00000000	6.26627901
C	-1.16084300	0.00000000	-3.49160701
H	-2.20752200	0.00000000	6.55427100
H	-2.20752200	0.00000000	-3.77959900
H	-0.65359499	-0.88873700	6.63730301

H	-0.65359500	0.88873701	-3.86263100
H	-0.65359500	0.88873701	6.63730300
H	-0.65359499	-0.88873700	-3.86263101
Na	-0.00026899	-2.35000000	1.38733600

$C_6H_4(COOH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.77007400
C	1.21328200	0.00000000	0.69133400
C	-1.21365400	0.00000000	0.68997200
C	-1.21365400	0.00000000	2.08010200
C	1.21328200	0.00000000	2.07874000
H	-2.14508699	0.00000000	0.14103500
H	2.13743600	0.00000000	0.12866400
H	-2.14508699	0.00000000	2.62903900
H	2.13743600	0.00000000	2.64141000
C	0.05128399	0.00000000	4.25748800
C	0.05128399	0.00000000	-1.48741400
O	1.06872100	0.00000000	4.90980300
O	1.06872100	0.00000000	-2.13972900
O	-1.16978700	0.00000000	4.82924500
O	-1.16978700	0.00000000	-2.05917100
H	-1.03022900	0.00000000	5.78995000
H	-1.03022900	0.00000000	-3.01987600
Na	-0.00012401	-2.40000000	1.38503700

$C_6H_4(COCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39959055
C	1.21385595	0.00000000	-0.69005244
C	2.41510048	0.00000000	1.40711957
C	2.41681640	0.00000000	0.01083317
C	1.19752390	0.00000000	2.09730865
C	3.68595567	0.00000000	2.20703404
O	3.64457635	0.00000000	3.42141834
C	-1.32259217	0.00000000	-0.71111603
O	-2.35864256	0.00000000	-0.07626089
C	-1.33663768	0.00000000	-2.22224184
C	5.00748892	0.00000000	1.47406178
H	-0.95094393	-0.00000000	1.91601074
H	1.23285053	0.00000000	-1.77230983
H	3.34896145	-0.00000000	-0.53939174
H	1.21720822	-0.00000000	3.17924982
H	-0.82574842	0.88346028	-2.61235346
H	-0.82574760	-0.88345951	-2.61235344
H	-2.37181018	0.00000000	-2.55567053
H	5.09492878	-0.88345951	0.83723370
H	5.09492920	0.88346028	0.83723441
H	5.80803714	0.00000000	2.21018633
Na	1.20721596	2.35000000	0.70413354

$C_6H_4(OCF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39047962
C	1.18654338	0.00000000	-0.71757477
C	2.39764620	0.00000000	1.35654146
C	2.40162903	0.00000000	-0.03010301
C	1.20576416	0.00000000	2.07267747
C	-1.43401113	-0.00000000	-1.90446754
C	4.76866093	-0.00000000	1.60488335
O	-1.27409773	-0.00000000	-0.56916155
O	3.54171236	-0.00000000	2.15552989
F	-0.88846886	-1.08104460	-2.48964171
F	-0.88846900	1.08104561	-2.48964034
F	-2.73741446	-0.00000000	-2.16070618
F	4.98928631	1.08104298	0.83587520
F	4.98928667	-1.08104722	0.83588154
F	5.65959112	0.00000418	2.59015583
H	-0.94362721	-0.00000000	1.91887007
H	1.19660117	-0.00000000	-1.79678457
H	3.32151883	-0.00000000	-0.59454758
H	1.23883644	0.00000000	3.15366544
Na	1.19859729	2.45000000	0.67866985

$C_6H_4(BF_2)_2\cdots Na^+$

C	0.69500700	1.20965400	0.00054965
C	-0.69500700	1.20965400	0.00054965
C	-0.69500700	-1.20965400	0.00054965
C	0.69500700	-1.20965400	0.00054965
C	1.40221200	0.00000000	0.00034665
C	-1.40221200	0.00000000	0.00034665
H	1.23828400	2.14683700	0.00031265
H	-1.23828400	2.14683700	0.00031265
H	-1.23828400	-2.14683700	0.00031265
H	1.23828400	-2.14683700	0.00031265
F	-3.64749100	1.13532100	-0.00046635
F	-3.64749100	-1.13532100	-0.00046635
F	3.64749100	1.13532100	-0.00046635
F	3.64749100	-1.13532100	-0.00046635
B	-2.95365200	0.00000000	-0.00018135
B	2.95365200	0.00000000	-0.00018135
Na	0.00000000	0.00000000	2.40054965

$C_6H_4(CHO)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40057430
C	1.19821055	0.00000000	-0.71309801
C	2.40756374	0.00000000	1.36921621
C	2.40789033	0.00000000	-0.02513567
C	1.20383837	0.00000000	2.08521454
C	3.70403325	0.00000000	2.09313895
O	3.80504942	0.00000000	3.29856963
C	-1.28495445	0.00000000	-0.74417028
O	-2.37260463	0.00000000	-0.21475129
H	-0.94908144	0.00000000	1.92164726
H	1.18148511	-0.00000000	-1.79757084
H	3.34849223	-0.00000000	-0.56516264
H	1.24118876	0.00000000	3.16728550
H	4.60294948	0.00000000	1.45233628
H	-1.19375763	0.00000000	-1.84433462
Na	1.20291683	2.40000000	0.68612913

$C_6H_4(CF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000

C	0.00000000	0.00000000	1.39017808
C	1.21182593	0.00000000	2.07581728
C	2.42365081	0.00160050	1.39017808
C	2.42365081	0.00160050	0.00000000
C	1.21182593	0.00000000	-0.68563920
H	-0.93380261	-0.00941515	-0.54615271
H	-0.93380261	-0.00941515	1.93633079
H	3.35746504	-0.00658134	1.93633079
H	3.35746504	-0.00658134	-0.54615271
C	1.21179363	0.04892249	-2.18688577
C	1.21179363	0.04892249	3.57706385
F	1.21095394	1.32046673	-2.63884073
F	0.12668212	-0.55193522	-2.70927606
F	2.29769776	-0.55050155	-2.70927606
F	1.21095394	1.32046673	4.02901881
F	0.12668212	-0.55193522	4.09945414
F	2.29769776	-0.55050155	4.09945414
Na	1.21126009	2.50055113	0.69708795

$C_6H_4(NO)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39031583
C	1.18413250	0.00000000	-0.74860402
C	2.39485518	0.00000000	1.31951914
C	2.39506924	0.00000000	-0.08140116
C	1.21957266	0.00000000	2.06227691
N	3.60936790	0.00000000	2.10759151
O	4.62243290	-0.00000000	1.45917431
N	-1.31502238	0.00000000	-0.60565282
O	-1.30810919	-0.00000000	-1.80844032
H	-0.94656196	0.00000000	1.91569618
H	1.12798536	0.00000000	-1.82889411
H	3.33827205	0.00000000	-0.61106866
H	1.28113845	0.00000000	3.14311626
Na	1.19893845	2.50000000	0.65701746

$C_6H_4(SiF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40042722
C	1.22056605	0.00000000	-0.68668526
C	2.42117000	0.02887003	1.41590634
C	2.42130733	0.01431764	0.01551128
C	1.20076718	0.01431795	2.10263891
Si	-1.58607304	-0.00271167	-0.92776058
F	-2.12240001	1.46440554	-1.25191172
F	-2.72699391	-0.73243642	-0.08535212
F	-1.41602832	-0.74824863	-2.32745647
Si	4.00714781	0.06398190	2.34316914
F	4.52644765	1.54368641	2.63635123
F	5.15681110	-0.66987408	1.51635667
F	3.84523266	-0.65406918	3.75810262
H	-0.93563386	-0.02218014	1.94677763
H	1.23804566	-0.02232314	-1.77005466
H	3.35723880	0.00294612	-0.53074514
H	1.18365596	0.00309027	3.18614368
Na	1.19123971	2.45950750	0.70796641

$C_6H_4(CN)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39871924
C	1.20102107	0.00000000	-0.71691276
C	2.40744937	-0.00248157	1.36668258
C	2.40745033	-0.00124358	-0.03203611
C	1.20642927	-0.00124358	2.08359589
C	-1.25198251	0.00050253	-0.71073673
C	3.65943065	-0.00456011	2.07741861
N	-2.25698554	0.00063348	-1.28126592
N	4.66443227	-0.00650105	2.64794700
H	-0.93838941	0.00192954	1.93650101
H	1.18182056	0.00192954	-1.79830781
H	3.34584198	-0.00030111	-0.56981661
H	1.22563201	-0.00030111	3.16499221
Na	1.20544630	2.49917062	0.68334147

$C_6H_4(NO_2)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38951400
C	2.44284400	0.00000000	1.38951400
C	2.44284400	0.00000000	-0.00000000
C	1.22142200	0.00000000	-0.66068000
C	1.22142200	0.00000000	2.05019400
O	0.14234300	0.00000000	4.08293100
O	2.30050100	0.00000000	4.08293100
O	0.14234300	0.00000000	-2.69341700
O	2.30050100	0.00000000	-2.69341700
N	1.22142200	0.00000000	3.52562800
N	1.22142200	0.00000000	-2.13611400
H	-0.92044400	0.00000000	-0.56480500
H	-0.92044400	0.00000000	1.95431900
H	3.36328800	0.00000000	1.95431900
H	3.36328800	0.00000000	-0.56480500
Na	1.22142200	2.60000000	0.69475700

$C_6H_4Cl_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39261400
C	1.21141000	0.00000000	2.07699100
C	2.42282000	0.00000000	1.39261400
C	2.42282000	0.00000000	0.00000000
C	1.21141000	0.00000000	-0.68437700
H	-0.93502000	0.00000000	-0.55015800
H	-0.93502000	0.00000000	1.94277200
H	3.35784001	0.00000000	1.94277200
H	3.35784001	0.00000000	-0.55015800
Cl	1.21141000	0.00000000	-2.42701100
Cl	1.21141000	0.00000000	3.81962500
Na	1.21141000	-2.40000000	0.69630700

$C_6H_4Br_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39171800
C	1.21035300	0.00000000	2.07680700
C	2.42070600	0.00000000	1.39171800
C	2.42070600	0.00000000	0.00000000

C	1.21035300	0.00000000	-0.68508900
H	-0.93655600	0.00000000	-0.54681300
H	-0.93655600	0.00000000	1.93853100
H	3.35726200	0.00000000	1.93853100
H	3.35726200	0.00000000	-0.54681300
Br	1.21035300	0.00000000	-2.56710000
Br	1.21035300	0.00000000	3.95881800
Na	1.21035300	-2.40000000	0.69585900

$C_6H_4(NC)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38801400
C	1.21574300	0.00000000	2.07512100
C	2.43148599	0.00000000	1.38801400
C	2.43148599	0.00000000	-0.00000000
C	1.21574300	0.00000000	-0.68710700
H	-0.92956800	-0.00000000	-0.55861300
H	-0.92956800	0.00000000	1.94662700
H	3.36105399	0.00000000	1.94662700
H	3.36105399	0.00000000	-0.55861300
N	1.21574300	0.00000000	-2.07324400
N	1.21574300	0.00000000	3.46125800
C	1.21574300	0.00000000	-3.24804900
C	1.21574300	0.00000000	4.63606300
Na	1.21574300	-2.45000000	0.69400700

$C_6H_3X_3\cdots Na^+$ geometries

$C_6H_3(CH_2OH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40033954
C	1.20321118	0.00000000	2.08999057
C	2.41594080	0.00000000	1.38982079
C	2.41159053	0.00000000	0.00298385
C	1.19886090	0.00000000	-0.69718593
H	-0.93231882	0.00000000	-0.55163941
H	3.35548368	0.00000000	-0.52860823
H	1.19163684	0.00000000	3.17322205
C	1.23619783	0.00000000	-2.20484718
C	3.70294528	0.00000000	2.17598615
C	-1.32434140	0.00000000	2.12183544
H	1.77866736	0.88664200	-2.54968823
H	1.77866736	-0.88664200	-2.54968823
H	-1.89421729	-0.88664200	1.82446356
H	-1.89421729	0.88664200	1.82446356
H	3.73035162	-0.88664200	2.81819908
H	3.73035162	0.88664200	2.81819908
O	4.80966447	0.00000000	1.28466329
H	5.62511283	0.00000000	1.79747627
O	-0.08907000	0.00000000	-2.71763268
H	-0.05268512	0.00000000	-3.68023817
O	-1.10579275	0.00000000	3.52594379
H	-1.95762600	0.00000000	3.97573631
Na	1.20493390	2.30000000	0.69765814

$C_6H_3(NHOH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40266330
C	1.18309269	0.00000000	2.12382694
C	2.39783431	0.00141125	1.42249545
C	2.43083390	0.00142500	0.03732579
C	1.21609231	0.00139975	-0.66400609
N	1.29337432	-0.06005801	-2.07442616
N	-1.26002852	-0.06292327	2.04094573
N	3.58068988	-0.06011168	2.19457239
O	0.09261499	0.32626367	-2.69856357
O	-1.20062059	0.32349265	3.39289533
O	4.72135513	0.32762845	1.46714243
H	-0.92635734	0.00478362	-0.55665110
H	1.16419150	0.00478091	3.20440172
H	3.37608330	0.00730446	-0.48659281
H	2.00596885	0.57046423	-2.42283945
H	-1.91879930	0.56681925	1.59801550
H	3.52574865	0.56958113	2.98653842
H	-0.16283171	-0.45253352	-3.20868753
H	-1.51376452	-0.45566356	3.86919516
H	5.29132723	-0.45085961	1.50019700
Na	1.20329411	2.30070560	0.72038432

$C_6H_3(N(CH_3)_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40397834
C	1.21984064	0.00000000	2.09906268
C	2.43533407	0.03368567	1.39720948
C	2.42753014	0.03357794	-0.00674710
C	1.21157173	0.03368569	-0.70860081
H	-0.93205581	-0.02363137	-0.53491404
H	3.35689617	0.03569372	-0.54683483
H	1.22315477	-0.02363094	3.17370227
N	1.20721125	0.06912270	-2.10122403
N	-1.20446258	0.00206993	2.10393501
N	3.64314944	0.06912312	2.09046141
C	-0.02236188	-0.26803662	-2.79060025
H	0.15287016	-0.22015720	-3.86358587
H	-0.80606240	0.45349209	-2.55511070
H	-0.38596969	-1.27336075	-2.53732364
C	-1.17752953	-0.33458107	3.51344078
H	-2.19535540	-0.31487560	3.89806777
H	-0.60198470	0.40310584	4.07452128
H	-0.74875015	-1.32844097	3.70166329
C	4.85927996	-0.23395062	1.36249270
H	5.70034783	-0.19101899	2.05173674
H	5.03702427	0.50899585	0.58359427
H	4.83545523	-1.22881492	0.89696448
C	2.44178852	-0.23395178	-2.79744912
H	2.83446458	-1.22881511	-2.54627441
H	3.20652876	0.50899516	-2.56626264
H	2.25933841	-0.19101950	-3.86944030
C	-2.41577165	-0.33458121	1.38271231
H	-2.36702692	-1.32844157	0.91698291
H	-2.61832345	0.40310548	0.60487130
H	-3.25386151	-0.31487606	2.07662389
C	3.63337217	-0.26803530	3.50006918

H	3.23329772	-1.27335996	3.69059562
H	3.04077135	0.45349311	4.06439706
H	4.65238518	-0.22015623	3.87903593
Na	1.17286974	2.26636376	0.70422608

$C_6H_3(NHCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40986263
C	1.20141657	0.00000000	2.11126596
C	2.42228953	0.01743041	1.40636995
C	2.42905576	0.01740161	0.01521065
C	1.20805888	0.01727683	-0.68968476
H	-0.94556384	0.01230061	-0.52582376
H	3.35705904	0.04329668	-0.54055090
H	1.21861111	0.01264526	3.19305950
N	1.25011452	0.06038802	-2.07769074
H	2.11452035	-0.27783746	-2.46722558
N	-1.22358812	0.02564251	2.06740428
H	-1.98819754	-0.32362298	1.51358216
N	3.60302068	0.06005939	2.13728967
H	3.51068644	-0.29047997	3.07639967
C	0.07092603	-0.24328421	-2.85932755
H	0.34843535	-0.26439644	-3.91232901
H	-0.67943112	0.53910086	-2.72953045
H	-0.38085866	-1.20699256	-2.59016850
C	-1.30659377	-0.27912307	3.47945433
H	-2.35687440	-0.31526142	3.76559669
H	-0.83028613	0.51022017	4.06432819
H	-0.83385111	-1.23613253	3.73623203
C	4.87165123	-0.22661710	1.50321381
H	5.64501207	-0.25160781	2.26973671
H	5.12869672	0.56642815	0.79821797
H	4.87138444	-1.18377614	0.96550242
Na	1.18681374	2.30875410	0.71259931

$C_6H_3(OCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40482013
C	1.18105126	0.00000000	2.12885713
C	2.39766176	0.00000000	1.42644772
C	2.43417046	0.00000000	0.04160804
C	1.21756088	0.00000000	-0.66080304
O	3.50862742	0.00000000	2.21226861
O	-1.23602344	0.00000000	1.97403264
O	1.34261960	-0.00000000	-2.01583680
C	4.76997859	0.00000000	1.56606650
C	-1.30707242	0.00000000	3.38949719
C	0.15231554	-0.00000000	-2.78509854
H	-0.95190647	-0.00000000	-0.50858580
H	1.21655646	0.00000000	3.20752542
H	3.35057266	0.00000000	-0.52847481
H	4.89163215	-0.89383700	0.94953885
H	4.89163215	0.89383700	0.94953885
H	5.51090270	0.00000000	2.36092141
H	-0.83397010	-0.89383700	3.80311614
H	-0.83397010	0.89383700	3.80311614
H	-2.36589795	0.00000000	3.63372840
H	-0.44243905	-0.89383700	-2.58218925
H	-0.44243905	0.89383700	-2.58218925
H	0.47021919	-0.00000000	-3.82418441
Na	1.20507422	2.30000000	0.72348827

$C_6H_3(OH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39451450
C	1.18401679	0.00000000	2.12282018
C	2.39170166	0.00000000	1.42556334
C	2.43042476	0.00000000	0.03602185
C	1.22274028	0.00000000	-0.66123490
O	3.52967040	0.00000000	2.17645270
O	-1.21927387	0.00000000	2.00458043
O	1.30404448	-0.00000000	-2.02218979
H	-0.94264329	-0.00000000	-0.53256835
H	1.19411978	0.00000000	3.20545791
H	3.36296453	0.00000000	-0.51404621
H	4.30208356	0.00000000	1.59793780
H	-1.10447208	0.00000000	2.96276640
H	0.41682915	-0.00000000	-2.40186177
Na	1.20481367	2.35000000	0.71961445

$C_6H_3(CH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39563423
C	1.22430999	0.00000000	2.06560439
C	2.43293428	0.00945169	1.36779775
C	2.40100310	0.00932717	-0.02747071
C	1.19234188	0.00945143	-0.72527653
H	-0.94647265	-0.01405840	-0.53215461
H	3.33513315	0.00257449	-0.58114081
H	1.23678700	-0.01405872	3.15134983
C	1.17498007	0.03592933	-2.23375101
C	3.74789706	0.03592971	2.10716765
C	-1.29786907	0.01632767	2.16489708
H	0.28779335	-0.46367784	-2.62576290
H	1.16676773	1.06540514	-2.60197044
H	2.05682000	-0.45680566	-2.64600250
H	-2.09195317	-0.48254199	1.60727635
H	-1.62064003	1.04331026	2.35620740
H	-1.18989781	-0.48254119	3.12918567
H	3.66589506	-0.46367775	3.07362892
H	4.06697214	1.06540490	2.29113407
H	4.53286635	-0.45680538	1.53148001
Na	1.20283701	2.30469975	0.68137043

$C_6H_3(NH_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39735815
C	1.20637436	0.00000000	2.10257894
C	2.41651628	0.00416298	1.40390239
C	2.42407046	0.00417526	0.00654049
C	1.21392183	0.00416427	-0.69213789
H	-0.93753990	0.02419090	-0.54460214
H	3.36443461	0.03160137	-0.53301674
H	1.20341972	0.02418985	3.18681361

N	1.21742905	0.06094326	-2.08716725
H	0.38396417	-0.29455999	-2.52889251
H	2.05426502	-0.29179121	-2.52468210
N	-1.21007506	0.05261642	2.09183358
H	-1.17466467	-0.30275914	3.03450127
H	-2.00617086	-0.30286772	1.58587101
N	3.62279717	0.06094127	2.10462073
H	4.42268655	-0.29168394	1.60262643
H	3.58389170	-0.29467015	3.04704554
Na	1.20858240	2.30251033	0.70675254

$C_6H_3(SCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40521444
C	1.19743839	0.00000000	2.10662566
C	2.41439028	0.00000000	1.40401939
C	2.42311113	0.00000000	0.01630160
C	1.20616008	0.00000000	-0.68630710
C	5.20256464	0.00000000	1.18017938
C	-1.20023674	0.00000000	3.93176444
C	-0.38177839	-0.00000000	-2.98901656
S	3.87408072	0.00000000	2.40707042
S	-1.59851426	0.00000000	2.16781812
S	1.34498253	-0.00000000	-2.45196214
H	-0.94694974	0.00000000	-0.52190060
H	1.21893430	0.00000000	3.18765955
H	3.34856495	0.00000000	-0.54283170
H	5.16965151	-0.89449000	0.55907936
H	5.16965151	0.89449000	0.55907936
H	6.13069948	0.00000000	1.74959937
H	-0.64589136	-0.89449000	4.21380992
H	-0.64589136	0.89449000	4.21380992
H	-2.15743549	0.00000000	4.45084258
H	-0.90320979	-0.89449000	-2.64996256
H	-0.90320979	0.89449000	-2.64996256
H	-0.35271309	-0.00000000	-4.07751437
Na	1.20684984	2.30000000	0.70764242

$C_6H_3(SH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39564325
C	1.20415778	0.00000000	2.10123202
C	2.41248314	0.02342200	1.40427628
C	2.42173745	0.06645842	0.00950510
C	1.21328059	0.04530823	-0.68819540
H	-0.93753790	-0.04772298	-0.54694715
H	3.35985526	0.13841755	-0.53386191
H	1.20109809	-0.02028890	3.18766464
S	3.91254641	0.08166261	2.35634420
S	-1.50150133	-0.08063225	2.34107571
S	1.29239287	0.04255917	-2.46304161
H	4.70518451	-0.45891993	1.41750577
H	0.00814368	0.37342671	-2.66796667
H	-2.31111523	0.36711468	1.36888165
Na	1.17168053	2.37215694	0.73586279

$C_6H_3(CCH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39811319
C	1.21169177	0.00000000	2.09562559
C	2.42249330	0.00000000	1.39656900
C	2.42071088	0.00000000	-0.00154304
C	1.20990934	0.00000000	-0.70059964
H	-0.93675882	0.00000000	-0.54004208
H	3.35678046	0.00000000	-0.54277895
H	1.21238101	0.00000000	3.17690358
C	1.20899440	0.00000000	-2.13594190
C	1.20822499	0.00000000	-3.34297186
H	1.20754567	0.00000000	-4.40868202
C	-1.24258539	0.00000000	2.11657668
C	-2.28751930	0.00000000	2.72075799
H	-3.21011170	0.00000000	3.25420138
C	3.66599363	0.00000000	2.11344777
C	4.71169694	0.00000000	2.71629642
H	5.63496867	0.00000000	3.24856318
Na	1.21080088	2.35000000	0.69802752

$C_6H_3(SiH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39980357
C	1.23416899	0.00000000	2.06031872
C	2.44635916	0.01485542	1.36044360
C	2.40132799	0.01458129	-0.03863665
C	1.18904711	0.01485574	-0.73851117
Si	4.08696243	0.05799038	2.27302884
Si	1.15858303	0.05799024	-2.61559971
Si	-1.61079910	0.02339158	2.36470341
H	-0.94944231	-0.01960898	-0.52808996
H	1.25176589	-0.01960915	3.14660105
H	3.33345893	0.00639884	-0.59700027
H	3.94419906	-0.63148072	3.58321307
H	4.52471605	1.45804213	2.52617485
H	5.12862240	-0.61668196	1.45321226
H	-0.06393490	-0.63148081	-3.10795406
H	1.14195037	1.45804093	-3.12100569
H	2.37291043	-0.61668339	-3.14716324
H	-2.67002370	-0.66403996	1.57869069
H	-2.05714837	1.41807293	2.63207534
H	-1.41760032	-0.66404029	3.66948253
Na	1.19780716	2.30733908	0.67390254

$C_6H_3F_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38578306
C	1.15476137	0.00000000	2.15188849
C	2.35488453	0.00000000	1.45899766
C	2.44097078	0.00000000	0.07589157
C	1.24084882	0.00000000	-0.61699992
F	1.28266754	0.00000000	-1.96207223
F	-1.18577668	0.00000000	2.02210215
F	3.49884129	0.00000000	2.16775013
H	-0.91811291	-0.00000000	-0.56882814
H	1.12119855	0.00000000	3.23141243
H	3.39264770	0.00000000	-0.43480349

Na	1.19857779	2.50000000	0.74259360

$C_6H_3(COOCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39496547
C	1.20196932	0.00000000	2.09871951
C	2.41004510	0.00000000	1.40123762
C	2.41852972	0.00000000	0.00842381
C	1.21045427	0.00000000	-0.68905839
C	1.27209679	-0.00000000	-2.17899301
O	2.30330060	-0.00000000	-2.81265267
O	0.05849237	-0.00000000	-2.74551723
C	3.66954508	0.00000000	2.19958893
O	3.70270872	0.00000000	3.40946651
O	4.76697167	-0.00000000	1.43183844
C	-1.32114250	0.00000000	2.08654877
O	-2.38550943	0.00000000	1.51033001
O	-1.20496329	-0.00000000	3.42082315
C	0.05671324	-0.00000000	-4.18172857
C	-2.44786995	0.00000000	4.14046903
C	6.01165661	0.00000000	2.14840339
H	-0.94244459	0.00000000	-0.52973657
H	1.21442619	0.00000000	3.17976965
H	3.34851829	0.00000000	-0.54288922
H	0.56330354	-0.88875400	-4.55237105
H	-0.99010931	-0.00000000	-4.46714355
H	0.56330354	0.88875400	-4.55237105
H	-3.02215156	-0.88875400	3.88707073
H	-2.17163519	-0.00000000	5.18975168
H	-3.02215156	0.88875400	3.88707073
H	6.78224440	-0.00000000	1.38453572
H	6.07934740	0.88875400	2.77244502
H	6.07934740	-0.88875400	2.77244502
Na	1.20683330	2.40000000	0.70238128

$C_6H_3(COOH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39510967
C	1.20024354	0.00000000	2.10109598
C	2.40844365	0.00000000	1.40354122
C	2.41972416	0.00000000	0.01110696
C	1.21152405	0.00000000	-0.68644795
C	1.27054725	-0.00000000	-2.17339247
O	2.29381397	-0.00000000	-2.81564611
O	0.05190972	-0.00000000	-2.74576084
C	3.66666372	0.00000000	2.19812914
O	3.71123887	0.00000000	3.40543058
O	4.77166851	-0.00000000	1.42894216
C	-1.31724327	0.00000000	2.08746627
O	-2.38508418	0.00000000	1.52241873
O	-1.20361053	-0.00000000	3.42902162
H	-0.94191793	0.00000000	-0.53129519
H	1.21108658	0.00000000	3.18246838
H	3.35079905	0.00000000	-0.53897024
H	0.18761800	-0.00000000	-3.70726458
H	5.53650051	0.00000000	2.02722070
H	-2.10415055	0.00000000	3.79224585

Na	1.20665589	2.45000000	0.70406765

$C_6H_3(COCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40023499
C	1.20933552	0.00000000	2.08597025
C	2.42197491	0.00000000	1.38585254
C	2.41117126	0.00000000	-0.00432908
C	1.19853169	0.00000000	-0.70444735
C	1.25037281	-0.00000000	-2.20478121
O	2.32399733	-0.00000000	-2.77515644
C	-1.32524676	0.00000000	2.10550708
O	-2.35601902	0.00000000	1.46090893
C	3.69538171	0.00000000	2.18091510
O	3.65252866	0.00000000	3.39588964
C	-0.04768125	-0.00000000	-2.97412768
C	-1.34249441	0.00000000	3.61432814
C	5.01068262	0.00000000	1.44144168
H	-0.95865834	0.00000000	-0.50221934
H	1.25372951	0.00000000	3.16730302
H	3.32543562	0.00000000	-0.58344252
H	-0.64215737	-0.88218800	-2.72594517
H	-0.64215737	0.88218800	-2.72594517
H	0.18178256	-0.00000000	-4.03694698
H	-0.83032344	-0.88218800	4.00506809
H	-0.83032344	0.88218800	4.00506809
H	-2.37765486	0.00000000	3.94701621
H	5.09298758	-0.88218800	0.80251825
H	5.09298758	0.88218800	0.80251825
H	5.81637908	0.00000000	2.17157194
Na	1.20683560	2.40000000	0.69388039

$C_6H_3(OCF_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39328319
C	1.16515090	0.00000000	2.13921361
C	2.37176947	0.00000000	1.44257067
C	2.43518848	0.00000000	0.06055600
C	1.22856919	0.00000000	-0.63608495
O	3.48225876	0.00000000	2.27446727
O	-1.27568801	0.00000000	1.93904708
O	1.39376791	-0.00000000	-2.01374545
C	4.73406136	0.00000000	1.76676898
C	-1.46190923	0.00000000	3.27698922
C	0.32818724	-0.00000000	-2.84398859
F	-0.92716882	-1.08105000	3.86658293
F	-0.92716882	1.08105000	3.86658293
F	-2.76892167	0.00000000	3.50218425
F	-0.44978648	-1.08105000	-2.67568734
F	-0.44978648	1.08105000	-2.67568734
F	0.78666907	-0.00000000	-4.08849214
F	5.58259196	0.00000000	2.78607749
F	4.97729467	1.08105000	1.00887402
F	4.97729467	-1.08105000	1.00887402
H	-0.94313930	-0.00000000	-0.52325298
H	1.18357009	0.00000000	3.21762262
H	3.35990788	0.00000000	-0.49459933

Na	1.20011313	2.50000000	0.73325654

$C_6H_3(BF_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39968734
C	1.22929073	0.00000000	2.06904301
C	2.44145552	0.00000000	1.36919934
C	2.40648918	0.00000000	-0.03007550
C	1.19432438	0.00000000	-0.72991917
H	-0.94595387	0.00000000	-0.53051395
H	3.33890466	0.00000000	-0.58403861
B	1.17496865	0.00000000	-2.27973031
H	1.24282910	0.00000000	3.15352006
B	-1.33249796	0.00000000	2.19135546
B	3.79330921	0.00000000	2.12734236
F	0.03010278	0.00000000	-2.95595768
F	2.30259122	0.00000000	-2.98433611
F	4.95137222	0.00000000	1.47397312
F	3.83970445	0.00000000	3.45619506
F	-1.34569509	0.00000000	3.52095208
F	-2.50651577	0.00000000	1.56710858
Na	1.21192792	2.45000000	0.67965507

$C_6H_3(CHO)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40090957
C	1.20212657	0.00000000	2.09592012
C	2.41535014	0.00000000	1.39546464
C	2.41618378	0.00000000	0.00688673
C	1.20296021	0.00000000	-0.69356736
C	1.20394630	-0.00000000	-2.17835841
O	2.21369479	-0.00000000	-2.84436943
C	-1.28635956	0.00000000	2.14244970
O	-2.36801641	0.00000000	1.60098888
C	3.70072328	0.00000000	2.13871461
O	3.77263196	0.00000000	3.34618740
H	-0.95054159	0.00000000	-0.52251467
H	1.22488616	0.00000000	3.18037027
H	3.34396484	0.00000000	-0.55504844
H	0.20895920	-0.00000000	-2.65403687
H	-1.20081564	0.00000000	3.24197457
H	4.61016806	0.00000000	1.51486977
Na	1.20610344	2.45000000	0.70093561

$C_6H_3(CF_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39067811
C	1.19261440	0.00000000	2.10597982
C	2.39697696	-0.00017873	1.41064076
C	2.42013922	-0.00018045	0.02015554
C	1.21577664	-0.00017873	-0.67518350
H	-0.93231486	0.01439523	-0.54867643
H	3.36146546	0.01407507	-0.51291644
H	1.18360624	0.01439523	3.18772641
C	1.22828909	-0.04070076	-2.17795630
C	3.69215708	-0.04070076	2.17286846
C	-1.30770166	-0.04032795	2.13122834
F	1.23198914	-1.30908270	-2.63356762
F	2.31852608	0.56303385	-2.68209231
F	0.14669028	0.56319546	-2.70017993
F	4.68526108	0.56303352	1.49721063
F	4.08478211	-1.30908270	2.40404146
F	3.58367887	0.56319578	3.36903178
F	-1.70431180	-1.30865105	2.35582810
F	-1.21907115	0.56355357	3.32903296
F	-2.28932471	0.56355389	1.43912419
Na	1.20435306	-2.60027424	0.70824166

$C_6H_3(NO)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40057966
C	1.18151274	0.00000000	2.12384647
C	2.39445035	0.00000000	1.42355582
C	2.43006168	0.00000000	0.03870222
C	1.21712407	0.00000000	-0.66158678
N	3.68638293	0.00000000	2.08033668
O	3.62678840	0.00000000	3.27994319
N	1.13994699	-0.00000000	-2.10882344
O	2.20863372	-0.00000000	-2.65701675
N	-1.21475551	0.00000000	2.19103547
O	-2.22384770	0.00000000	1.53962227
H	-0.92904183	0.00000000	-0.55600635
H	1.16451865	0.00000000	3.20642234
H	3.37609760	0.00000000	-0.48786730
Na	1.20385814	2.60000000	0.72084957

$C_6H_3(SiF_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39939290
C	1.22562422	0.00000000	2.07477608
C	2.43749380	-0.01073490	1.37509471
C	2.40959768	-0.01061172	-0.02401980
C	1.19768060	-0.01073472	-0.72370120
H	-0.94477647	0.02560599	-0.53309709
H	3.34374844	0.00672020	-0.57584678
H	1.23655005	0.02560657	3.15952352
Si	4.03928420	-0.01918322	2.27873968
Si	1.17931109	-0.01918409	-2.56271528
Si	-1.58347134	0.00557876	2.33479008
F	1.16673743	-1.49083950	-3.17392688
F	2.47785637	0.71004893	-3.12866666
F	-0.12378573	0.72150613	-3.10273230
F	-2.71639689	0.74474228	1.49311530
F	-2.11945283	-1.46138595	2.65140856
F	-1.39309070	0.74474322	3.73325044
F	3.88333602	0.72150626	3.68065264
F	4.56853127	-1.49083922	2.58473953
F	5.16167193	0.71004913	1.41458315
Na	1.20608690	-2.55539093	0.70212794

$C_6H_3(CN)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39562423
C	1.19943947	0.00000000	2.10914404

C	2.40808611	0.00000000	1.41133269
C	2.42629205	0.00000000	0.01582707
C	1.21764663	0.00000000	-0.68198509
C	1.22703408	0.00000000	-2.12103194
N	1.23456850	0.00000000	-3.27612081
C	-1.25094450	0.00000000	2.10701851
N	-2.25504838	0.00000000	2.67803730
C	3.64964316	0.00000000	2.13898526
N	4.64621262	0.00000000	2.72305534
H	-0.93311905	0.00000000	-0.54688302
H	1.19238447	0.00000000	3.19069164
H	3.36646732	0.00000000	-0.51883679
Na	1.20857758	2.60000000	0.70832394

$C_6H_3(NO_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38649240
C	1.16205994	0.00000000	2.14278364
C	2.36279693	0.00000000	1.44953751
C	2.43673504	0.00000000	0.06501858
C	1.23599805	0.00000000	-0.62822770
N	3.62021700	0.00000000	2.22094429
O	3.52491752	0.00000000	3.43011915
O	4.65496337	0.00000000	1.58810484
N	-1.29676676	0.00000000	2.08974623
O	-1.26608581	0.00000000	3.30228284
O	-2.29629418	0.00000000	1.40262721
N	1.27534595	0.00000000	-2.10288757
O	0.20991742	0.00000000	-2.68258547
O	2.37017164	0.00000000	-2.62494414
H	-0.92084442	-0.00000000	-0.56492309
H	1.13324480	0.00000000	3.22271919
H	3.38639459	0.00000000	-0.44999388
Na	1.19959833	2.75000000	0.73593407

$C_6H_3Cl_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39141145
C	1.18092862	0.00000000	2.12723304
C	2.38592657	0.00000000	1.43152744
C	2.43270248	0.00000000	0.04090216
C	1.22770454	0.00000000	-0.65480370
H	-0.92956513	-0.00000000	-0.55772820
H	1.16270476	0.00000000	3.21112416
H	3.38049147	0.00000000	-0.48526077
Cl	1.25692796	-0.00000000	-2.39289615
Cl	-1.51984386	0.00000000	2.23514934
Cl	3.87654701	0.00000000	2.32588200
Na	1.20454370	2.40000000	0.72271173

$C_6H_3Br_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39006118
C	1.17880355	0.00000000	2.12673768
C	2.38263064	0.00000000	1.43170674
C	2.43121083	0.00000000	0.04249490
C	1.22738200	0.00000000	-0.65253436
H	-0.92877310	0.00000000	-0.55809262
H	1.15986643	0.00000000	3.21012507
H	3.37891931	0.00000000	-0.48279890
Br	3.99485892	0.00000000	2.40048399
Br	-1.64509923	0.00000000	2.30190322
Br	1.26025295	-0.00000000	-2.53315365
Na	1.20333784	2.40000000	0.72307769

$C_6H_3(NC)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39406004
C	1.18771654	0.00000000	2.12394553
C	2.39500822	0.00000000	1.42691576
C	2.43324925	0.00000000	0.03337996
C	1.22595757	0.00000000	-0.66365031
H	-0.93099236	-0.00000000	-0.55467323
H	1.17285115	0.00000000	3.20754517
H	3.37910700	0.00000000	-0.49554645
N	1.24494576	-0.00000000	-2.04777756
N	3.58420379	0.00000000	2.13542312
N	-1.20818288	0.00000000	2.06967943
C	-2.23386539	0.00000000	2.64324409
C	1.26106565	-0.00000000	-3.22282664
C	4.59376640	0.00000000	2.73690754
Na	1.20698889	2.55000000	0.71910834

$C_6H_2X_4\cdots Na^+$ geometries

$C_6H_2(OH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39554797
C	1.20941957	0.00000000	2.08189733
C	2.40491069	0.00000000	1.37293722
C	2.40491069	0.00000000	-0.02261075
C	1.19549112	0.00000000	-0.70896011
H	1.19553387	0.00000000	3.16856592
H	1.20937683	-0.00000000	-1.79562871
O	3.57431554	0.00000000	-0.72162181
H	4.30795918	0.00000000	-0.08562654
O	3.65091698	0.00000000	1.95594046
H	3.57511387	0.00000000	2.91971735
O	-1.16940485	0.00000000	2.09455903
H	-1.90304849	0.00000000	1.45856376
O	-1.24600629	0.00000000	-0.58300324
H	-1.17020318	0.00000000	-1.54678013
Na	1.20245534	-2.35000000	0.68646861

$C_6H_2(CH_3)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39493000
C	1.17590772	0.00000000	2.14529181
C	2.40532428	0.00056046	1.47141455
C	2.40534145	0.00056047	0.07649455
C	1.22943545	0.00056047	-0.67388855
C	1.28213455	0.00072455	-2.18057720
C	-1.29847470	-0.00016430	-0.76608191

C	3.70380264	0.00072381	2.23747057
C	1.12318324	-0.00016408	3.65197957
H	-0.95250963	-0.00011903	1.91701961
H	3.35784437	0.00068049	-0.44560728
H	2.31466631	0.00172551	-2.53200806
H	0.78444422	-0.87972363	-2.59683813
H	0.78280271	0.88030810	-2.59670014
H	-1.38165152	0.88028577	-1.40954683
H	-1.38065082	-0.87974629	-1.41086128
H	-2.15015374	-0.00116719	-0.08472555
H	3.78700695	-0.87973037	2.88092632
H	4.55547457	0.00173876	1.55610534
H	3.78599692	0.88029732	2.88225919
H	1.62251106	-0.87974041	4.06812259
H	1.62085327	0.88028695	4.06825873
H	0.09065736	-0.00117410	4.00339667
Na	1.20213202	2.30028018	0.73570713

$C_6H_2(NH_2)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39325679
C	1.22117121	0.00000000	2.07900218
C	2.41038326	-0.01387642	1.35308909
C	2.41025445	-0.01342448	-0.04024939
C	1.18915433	-0.01169537	-0.72595422
N	3.59663633	-0.06175933	-0.80642480
N	1.22593371	0.02060432	-2.13858206
N	-1.18693180	0.04191156	2.16032133
N	1.18529977	-0.03438309	3.49063555
H	-0.94709156	-0.01248890	-0.53139417
H	3.35757692	-0.00285713	1.88428804
H	3.58195715	0.61488034	-1.56173566
H	4.42782221	0.06721482	-0.24692288
H	1.87227543	-0.66662578	-2.51092679
H	0.31430882	-0.10705524	-2.55483765
H	-2.01840186	-0.06590531	1.59675082
H	-1.18030441	-0.65379974	2.89834506
H	2.09397134	0.10753963	3.90848223
H	0.52413123	0.63755509	3.86440111
Na	1.21756450	2.29346684	0.67652391

$C_6H_2(SH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40360373
C	1.21111846	0.00000000	2.09362494
C	2.43448607	0.01017246	1.42266704
C	2.43431337	-0.03035894	0.01964864
C	1.22315398	-0.03996585	-0.67023383
H	1.18531103	-0.00694043	3.17994349
H	1.24876767	-0.07849227	-1.75589576
S	3.93875982	0.00564143	-0.93368527
H	4.55832949	-0.98431618	-0.26358562
S	3.98394153	0.05921677	2.28500209
H	3.45360511	-0.12488756	3.50467697
S	-1.50396781	0.07633089	2.35531540
H	-2.13203178	-0.92724952	1.71400565
S	-1.54908746	0.03732191	-0.86358232
H	-1.02048892	-0.18643753	-2.07736699
Na	1.23895418	2.35059488	0.64053201

$C_6H_2(CCH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39552780
C	1.19263607	0.00000000	2.12017740
C	2.42345035	0.00000000	1.42782331
C	2.42345035	0.00000000	0.03229551
C	1.23081429	0.00000000	-0.69235410
C	1.27023427	0.00000000	-2.12280688
C	1.32067290	0.00000000	-3.32863050
C	-1.24295285	-0.00000000	-0.70909612
C	-2.29965632	-0.00000000	-1.29213336
C	3.66640320	0.00000000	2.13691943
C	4.72310668	0.00000000	2.71995666
C	1.15321609	0.00000000	3.55063018
C	1.10277745	0.00000000	4.75645380
H	-0.94247567	0.00000000	1.92568649
H	3.36592603	0.00000000	-0.49786319
H	1.35491268	0.00000000	-4.39379648
H	-3.22774046	-0.00000000	-1.81597567
H	5.65119082	0.00000000	3.24379897
H	1.06853767	0.00000000	5.82161978
Na	1.21172518	2.35000000	0.71391165

$C_6H_2F_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38494046
C	1.21802730	0.00000000	2.04408353
C	2.41014391	0.00000000	1.33372578
C	2.41014391	0.00000000	-0.05121468
C	1.19211661	0.00000000	-0.71035775
F	1.15430518	0.00000000	-2.05006186
F	-1.16024701	-0.00000000	-0.67086785
F	3.57039092	0.00000000	2.00459363
F	1.25583873	0.00000000	3.38378763
H	-0.92875230	0.00000000	1.93836484
H	3.33889621	0.00000000	-0.60463906
Na	1.20507196	2.55000000	0.66686289

$C_6H_2(NO)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.46004792
C	1.28429983	0.00000000	2.13079137
C	2.42265602	0.00000000	1.41140474
C	2.42265602	0.00000000	-0.04864318
C	1.13835619	0.00000000	-0.71938663
H	1.29576134	0.00000000	3.21889373
H	1.12689468	-0.00000000	-1.80748899
N	3.52583191	0.00000000	-0.73513396
O	3.73991864	0.00000000	-1.92482186
N	3.65389545	0.00000000	2.16526384
O	4.64344439	0.00000000	1.49369340
N	-1.10317589	0.00000000	2.14653870
O	-1.31726262	0.00000000	3.33622660
N	-1.23123944	0.00000000	-0.75385910

O	-2.22078837	0.00000000	-0.08228865
Na	1.21132801	-2.55000000	0.70570237

$C_6H_2(CN)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39325600
C	1.20780255	0.00000000	2.08778843
C	2.42495001	0.00000000	1.38365874
C	2.42495001	0.00000000	-0.00959726
C	1.21714747	0.00000000	-0.70412969
C	1.22903419	0.00000000	-2.14099207
N	1.25766919	0.00000000	-3.29545057
C	-1.25153005	-0.00000000	-0.70596553
N	-2.26659538	-0.00000000	-1.25663493
C	1.19591582	0.00000000	3.52465081
N	1.16728083	0.00000000	4.67910932
C	3.67648007	0.00000000	2.08962427
N	4.69154539	0.00000000	2.64029367
H	-0.93584507	0.00000000	1.93464997
H	3.36079509	0.00000000	-0.55099123
Na	1.21247501	2.75000000	0.69182937

$C_6H_2Cl_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39714400
C	1.20792800	0.00000000	2.08705800
C	2.41585600	0.00000000	1.39714400
C	2.41585600	0.00000000	-0.00000000
C	1.20792800	0.00000000	-0.68991400
H	1.20792800	0.00000000	3.17163900
H	1.20792800	0.00000000	-1.77449500
Cl	3.89127000	0.00000000	-0.90161000
Cl	3.89127000	0.00000000	2.29875400
Cl	-1.47541400	0.00000000	-0.90161000
Cl	-1.47541400	0.00000000	2.29875400
Na	1.20792800	-2.45000000	0.69857200

$C_6H_2Br_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39458400
C	1.20901000	0.00000000	2.08036700
C	2.41802000	0.00000000	1.39458400
C	2.41802000	0.00000000	-0.00000000
C	1.20901000	0.00000000	-0.68578300
H	1.20901000	0.00000000	3.16440700
H	1.20901000	0.00000000	-1.76982300
Br	4.00204100	0.00000000	-0.99958300
Br	4.00204100	0.00000000	2.39416700
Br	-1.58402100	0.00000000	2.39416700
Br	-1.58402100	0.00000000	-0.99958300
Na	1.20901000	-2.45000000	0.69729200

$C_6H_2(NC)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40630400
C	1.20400100	0.00000000	2.10377700
C	2.40800200	0.00000000	1.40630400
C	2.40800200	0.00000000	0.00000000
C	1.20400100	0.00000000	-0.69747300
H	1.20400100	0.00000000	3.18772000
H	1.20400100	-0.00000000	-1.78141600
N	3.60213499	0.00000000	-0.68168300
N	3.60213499	0.00000000	2.08798700
N	-1.19413300	0.00000000	-0.68168300
N	-1.19413300	0.00000000	2.08798700
C	4.63518399	0.00000000	-1.24555400
C	4.63518399	0.00000000	2.65185800
C	-2.22718199	0.00000000	-1.24555400
C	-2.22718199	0.00000000	2.65185800
Na	1.20400100	-2.60000000	0.70315200

$C_6X_6\cdots Na^+$ geometries

$C_6(OH)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38992000
C	1.20370600	0.00000000	2.08488000
C	2.40741199	0.00000000	1.38992000
C	2.40741199	0.00000000	-0.00000000
C	1.20370600	0.00000000	-0.69496000
O	3.56228199	0.00000000	-0.73552900
H	4.31899399	0.00000000	-0.12709600
O	3.62183399	0.00000000	2.02230200
H	3.47327099	0.00000000	2.98185100
O	1.26325800	0.00000000	3.45279199
H	0.35798299	0.00000000	3.80390599
O	-1.15487000	0.00000000	2.12544900
H	-1.91158200	0.00000000	1.51701600
O	-1.21442200	0.00000000	-0.63238200
H	-1.06585900	0.00000000	-1.59193100
O	1.14415400	0.00000000	-2.06287199
H	2.04942900	0.00000000	-2.41398599
Na	1.20370600	2.35000000	0.69496000

$C_6(CH_3)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40284955
C	1.21528477	0.00000000	2.10361511
C	2.42828590	0.07444378	1.40284944
C	2.42828590	0.07444377	-0.00000011
C	1.21300113	0.07444378	-0.70076567
C	3.73547844	0.18066194	2.16037114
H	4.47252679	0.74948351	1.59462493
H	4.16837571	-0.80276863	2.37518825
H	3.59845195	0.69584083	3.11046616
C	1.21854080	-0.10621929	3.61443658
H	1.18839229	0.87721057	4.09676131
H	2.11005453	-0.62139796	3.97033095
H	0.36026007	-0.67504138	3.97033126
C	-1.31124408	0.02594554	2.16037190
H	-2.08175158	0.54855165	1.59462561
H	-1.20603188	0.54855039	3.11046648
H	-1.68308669	-0.98215507	2.37518968

C	-1.30719255	-0.10621817	-0.75752170
H	-1.74008981	0.87721241	-0.97233882
H	-2.04424090	-0.67503974	-0.19177550
H	-1.17016604	-0.62139706	-1.70761673
C	1.20974510	0.18066305	-2.21158714
H	0.31823137	0.69584174	-2.56748150
H	1.23989361	-0.80276680	-2.69391187
H	2.06802584	0.74948516	-2.56748182
C	3.73952997	0.04849823	-0.75752246
H	4.11137259	1.05659885	-0.97234025
H	3.63431777	-0.47410661	-1.70761705
H	4.51003748	-0.47410787	-0.19177617
Na	1.36170707	-2.20926068	0.65304521

$C_6(NH_2)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39530399
C	1.20989410	0.00000000	2.09030717
C	2.41063516	0.14853186	1.39530284
C	2.41063603	0.14853184	-0.00000065
C	1.20074193	0.14853184	-0.69500383
N	1.19578889	0.22890574	-2.11499658
N	-1.22883536	-0.08037272	-0.71159474
N	1.21484714	-0.08037390	3.51029992
N	3.63947139	0.22890456	2.10689808
N	3.64004349	0.21962301	-0.71159552
N	-1.22940746	-0.07109117	2.10689886
H	0.35438336	0.68819748	-2.44372429
H	1.97444611	0.78801762	-2.44372514
Na	1.06387128	2.36991241	0.69765167
H	-1.09477696	-0.53966414	-1.60493349
H	-1.90173233	-0.63948456	-0.20014778
H	0.43618904	-0.63948576	3.83902798
H	2.05625179	-0.53966463	3.83902720
H	4.31236749	0.78801642	1.59545062
H	3.50541213	0.68819600	3.00023633
H	4.37648797	-0.25265130	-0.20014867
H	3.56338159	-0.25265189	-1.60493533
H	-1.15274643	0.40118375	3.00023817
H	-1.96585282	0.40118415	1.59545158

$C_6(SH)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40691057
C	1.22606652	0.00000000	2.09709030
C	2.44292270	0.03672115	1.39537673
C	2.44292270	0.03672115	-0.01153384
C	1.21685618	0.03672115	-0.70171356
S	1.17185195	0.02093824	-2.48486964
H	2.19413545	0.87605596	-2.66339873
S	3.92303829	-0.01041167	-0.99507604
H	4.77112409	-0.19989315	0.02732452
S	3.99641423	0.15897018	2.26659246
H	3.68629743	-0.71484818	3.24073114
S	1.27107075	0.01578291	3.88024637
H	0.24878725	-0.83933481	4.05877547
S	-1.48011559	0.04713282	2.39045278
H	-2.32820139	0.23661430	1.36805221
S	-1.55349153	-0.12224903	-0.87121572
H	-1.24337473	0.75156933	-1.84535441
Na	1.18574188	2.36808899	0.69838723

$C_6(CCH)_6\cdots Na^+$

C	-1.21953110	-0.70409661	0.00000000
C	-1.21953110	0.70409661	0.00000000
C	0.00000000	1.40819321	0.00000000
C	1.21953110	0.70409661	0.00000000
C	1.21953110	-0.70409661	0.00000000
C	0.00000000	-1.40819321	0.00000000
C	0.00000000	2.83596068	0.00000000
C	0.00000000	4.04220007	0.00000000
H	0.00000000	5.10783027	0.00000000
C	-2.45601399	1.41798034	0.00000000
C	-3.50064795	2.02110004	0.00000000
H	-4.42351077	2.55391514	0.00000000
C	-2.45601399	-1.41798034	0.00000000
C	-3.50064795	-2.02110004	0.00000000
H	-4.42351077	-2.55391514	0.00000000
C	0.00000000	-2.83596068	0.00000000
C	0.00000000	-4.04220007	0.00000000
H	0.00000000	-5.10783027	0.00000000
C	2.45601399	-1.41798034	0.00000000
C	3.50064795	-2.02110003	0.00000000
H	4.42351077	-2.55391513	0.00000000
C	2.45601399	1.41798034	0.00000000
C	3.50064795	2.02110004	0.00000000
H	4.42351077	2.55391514	0.00000000
Na	0.00000000	0.00000000	2.40000000

$C_6F_6\cdots Na^+$

C	0.00000000	-1.38796700	0.00000000
C	-1.20201468	-0.69398350	0.00000000
C	-1.20201468	0.69398350	0.00000000
C	0.00000000	1.38796700	0.00000000
C	1.20201468	0.69398350	0.00000000
C	1.20201468	-0.69398350	0.00000000
F	-2.35488790	1.35959517	0.00000000
F	0.00000000	2.71919033	0.00000000
F	2.35488790	1.35959517	0.00000000
F	2.35488790	-1.35959517	0.00000000
F	0.00000000	-2.71919033	0.00000000
F	-2.35488790	-1.35959517	0.00000000
Na	0.00000000	0.00000000	2.70000000

$C_6(NO)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39443168
C	1.29557093	0.00000000	1.98520536
C	2.45372830	0.00000000	1.12917281
C	2.45372830	0.00000000	-0.26525887
C	1.15815736	0.00000000	-0.85603254
N	3.69534130	0.00000000	-0.97844929
O	3.54005420	-0.00000000	-2.17642284
N	3.51926266	0.00000000	1.98681116

O	4.71750990	0.00000000	1.82656873
N	-1.24161300	0.00000000	2.10762210
O	-1.08632591	-0.00000000	3.30559566
N	-1.06553436	-0.00000000	-0.85763835
O	-2.26378161	-0.00000000	-0.69739591
N	0.80876350	0.00000000	-2.13286242
O	-0.55549791	-0.00000000	-2.12460161
N	1.64496479	0.00000000	3.26203524
O	3.00922620	-0.00000000	3.25377443
Na	1.22686415	3.10000000	0.56458641

$C_6Cl_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39970768
C	1.21179808	0.00000000	2.09937983
C	2.42401532	0.00000000	1.39958631
C	2.42401532	0.00000000	-0.00012137
C	1.21221723	0.00000000	-0.69979352
Cl	3.91491836	0.00000000	-0.86134099
Cl	3.91537624	0.00000000	2.26067341
Cl	-1.49136093	0.00000000	-0.86108710
Cl	-1.49090304	0.00000000	2.26092730
Cl	1.21268945	0.00000000	-2.42156322
Cl	1.21132587	0.00000000	3.82114952
Na	1.21200766	-2.50000000	0.69979315

$C_6Br_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39821362
C	1.21069553	0.00000000	2.09585446
C	2.42040851	0.00000000	1.39471551
C	2.42040851	0.00000000	-0.00349811
C	1.20971298	0.00000000	-0.70113895
Br	4.03891154	0.00000000	-0.93440731
Br	4.03776214	0.00000000	2.32668555
Br	-1.61850303	0.00000000	2.32912283
Br	-1.61735363	0.00000000	-0.93197003
Br	1.20351753	0.00000000	-2.56825052
Br	1.21689098	0.00000000	3.96296604
Na	1.21020426	-2.45000000	0.69735776

$C_6(NC)_6\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40237504
C	1.21458358	0.00000000	2.10335053
C	2.42884671	0.00000000	1.40176603
C	2.42884671	0.00000000	-0.00060901
C	1.21426313	0.00000000	-0.70158450
N	3.61218369	0.00000000	-0.68318743
N	3.61203824	0.00000000	2.08462414
N	-1.18319153	-0.00000000	-0.68285812
N	-1.18333698	-0.00000000	2.08495345
C	4.63363139	0.00000000	-1.27137420
C	4.63294728	0.00000000	2.67382378
C	-2.20410057	-0.00000000	-1.27205776
C	-2.20478468	-0.00000000	2.67314022
N	1.21327831	0.00000000	-2.06767335
N	1.21556840	0.00000000	3.46943937
C	1.21155383	0.00000000	-3.24636588
C	1.21729288	0.00000000	4.64813191
Na	1.21442335	-3.00000000	0.70088301

$C_4H_2N_2X_2\cdots Na^+$ geometries

$C_4H_2N_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39566800
N	1.12982100	0.00000000	2.10344100
C	2.25964200	0.00000000	1.39566800
C	2.25964200	0.00000000	0.00000000
N	1.12982100	0.00000000	-0.70777300
H	-0.93257500	0.00000000	-0.55840300
H	-0.93257500	0.00000000	1.95407100
H	3.19221700	0.00000000	1.95407100
H	3.19221700	0.00000000	-0.55840300
Na	1.12982100	-2.50000000	0.69783400

$C_4H_2N_2(CH_2OH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39664133
N	1.12968226	0.00000000	2.09986315
C	2.27696433	0.00098329	1.41942009
C	2.27696433	0.00098329	0.02277876
N	1.14728208	0.00098329	-0.68044306
H	-0.93250656	0.00470418	1.95730384
H	3.20947089	-0.00372089	-0.53788375
C	3.54637691	0.04420704	2.24157135
H	4.34314731	-0.50735769	1.73300604
H	3.87108640	1.09353704	2.32733469
C	-1.26941258	-0.04322374	-0.82215126
H	-1.59412207	-1.09255374	-0.90791461
H	-2.06618298	0.50834098	-0.31358595
O	3.36983009	-0.52807953	3.51057888
H	2.45475966	-0.34656253	3.78429249
O	-1.09286576	0.52906282	-2.09115879
H	-0.17779533	0.34754582	-2.36487240
Na	1.13968268	-2.49950806	0.70951610

$C_4H_2N_2(NHOH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39986207
N	1.14096148	0.00000000	2.08154243
C	2.27332666	-0.01469678	1.38516580
C	2.27334096	0.01259791	-0.01443015
N	1.13238708	0.02708522	-0.69596926
H	-0.92551863	0.02367961	1.96415049
H	3.19888967	0.04630557	-0.57815905
N	-1.17984930	-0.08937480	-0.76189757
H	-1.05755247	0.40148483	-1.64597335
N	3.45307385	-0.12014670	2.14516383
H	3.33128251	0.35350969	3.03864364
O	4.54703425	0.47403223	1.48750102
H	5.20930059	-0.23146095	1.45216396

O	-2.27319308	0.49301420	-0.09276323
H	-2.93619882	-0.21233937	-0.07118191
Na	1.13792717	2.40415866	0.71609508

$C_4H_2N_2(N(CH_3)_2)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40926347
N	1.12201694	0.00000000	2.11689500
C	2.29048345	-0.00411988	1.46676611
C	2.28906666	-0.07918984	0.05950422
N	1.16713675	-0.07457830	-0.64825027
H	-0.92023649	-0.01388907	1.98434102
H	3.20754645	-0.15838112	-0.51309154
N	-1.16221340	0.08010142	-0.75744664
N	3.45565156	0.07233719	2.22003845
C	-1.08934356	-0.39264360	-2.13070283
H	-1.00050151	-1.48957088	-2.18757886
H	-1.99747760	-0.08150133	-2.65240273
H	-0.22405397	0.04599711	-2.62544817
C	-2.41953718	-0.15480298	-0.07827133
H	-2.49210398	-1.16962476	0.34848266
H	-2.56478540	0.57290699	0.72549192
H	-3.23259481	-0.02133495	-0.79469386
C	4.70254060	-0.24565349	1.55560492
H	4.73636227	-1.28378066	1.18358847
H	4.87431614	0.43221279	0.71436494
H	5.52077239	-0.10496376	2.26471761
C	3.36638904	-0.32350048	3.61645356
H	4.28613312	-0.01947288	4.12175126
H	2.51875179	0.17318590	4.08626038
H	3.23630709	-1.41170963	3.73159164
Na	1.18945158	2.32441266	0.67117580

$C_4H_2N_2(NHCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41952356
N	1.16920244	0.00000000	2.09752590
C	2.30138541	-0.03903328	1.38434371
C	2.30037489	-0.07882054	-0.03462179
N	1.13219693	-0.03848351	-0.71318990
H	-0.93160589	0.03811946	-0.56927871
H	3.23413036	-0.03230361	1.95299336
N	-1.16418052	-0.02684952	2.17782551
H	-1.00596796	0.23737908	3.14657253
N	3.46115227	-0.18596464	-0.79104433
H	3.31586441	0.05869662	-1.76692909
C	4.76090466	0.16066423	-0.22863565
H	5.51417607	0.08890226	-1.02515530
H	4.78553132	1.18277254	0.20214210
H	5.03435995	-0.55455669	0.56444726
C	-2.44506543	0.36939902	1.60499716
H	-2.75503238	-0.35296913	0.83207801
H	-3.20044098	0.35831385	2.40267883
H	-2.41809199	1.37896377	1.14572297
Na	1.06991756	-2.37643427	0.70344589

$C_4H_2N_2(OCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39909649
N	1.13874236	0.00000000	2.08620876
C	2.26687203	0.00000000	1.38866164
C	2.26687203	0.00000000	-0.01043485
N	1.12812967	0.00000000	-0.69754713
H	-0.93476301	0.00000000	1.95217328
H	3.20163504	0.00000000	-0.56351164
O	-1.19354443	0.00000000	-0.62800453
O	3.46041646	0.00000000	2.01666617
C	-1.16473793	0.00000000	-2.04978903
H	-0.65297611	0.88982400	-2.42725180
H	-0.65297611	-0.88982400	-2.42725180
H	-2.20920838	0.00000000	-2.35954435
C	3.43160996	0.00000000	3.43845067
H	2.91984814	0.88982400	3.81591344
H	2.91984814	-0.88982400	3.81591344
H	4.47608041	0.00000000	3.74820598
Na	1.13343601	2.40000000	0.69433082

$C_4H_2N_2(OH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39736727
N	1.14565673	0.00000000	2.07426699
C	2.26923228	0.00000000	1.37253175
C	2.26923228	0.00000000	-0.02483552
N	1.12357555	0.00000000	-0.70173524
H	-0.92981678	0.00000000	1.95734466
H	3.19904906	0.00000000	-0.58481290
O	-1.18054848	0.00000000	-0.65707972
O	3.44978075	0.00000000	2.02961147
H	-0.98445919	0.00000000	-1.60863997
H	3.25369146	0.00000000	2.98117173
Na	1.13461614	2.50000000	0.68626588

$C_4H_2N_2(CH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39975865
N	1.15640739	0.00000000	2.06935218
C	2.27351813	0.00000000	1.34693249
C	2.27351813	0.00000000	-0.05282616
N	1.11711074	0.00000000	-0.72241969
H	-0.93821068	0.00000000	-0.55142789
H	3.21172881	0.00000000	1.89836038
C	3.54552865	0.00000000	-0.85125546
H	3.58605022	-0.88235300	-1.49696716
H	3.58605022	0.88235300	-1.49696716
H	4.42429615	0.00000000	-0.20132041
C	-1.27201052	0.00000000	2.19818795
H	-1.31253209	-0.88235300	2.84389965
H	-1.31253209	0.88235300	2.84389965
H	-2.15077802	0.00000000	1.54825290
Na	1.13675906	-2.40000000	0.67346624

$C_4H_2N_2(NH_2)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40215022

N	1.15123337	0.00000000	2.07527340
C	2.27573854	-0.01255474	1.36956567
C	2.27577334	-0.00145088	-0.03254058
N	1.12457929	0.01109496	-0.70561408
H	-0.93362979	-0.00708378	-0.55927956
H	3.20929173	-0.02991864	1.92874843
N	3.45546819	-0.06656595	-0.77014196
H	3.32305634	0.20115356	-1.73845160
H	4.25573608	0.38884600	-0.35015072
N	-1.18009809	-0.06355929	2.13924209
H	-1.04603495	0.19564848	3.10963819
H	-1.97748558	0.40017104	1.72289037
Na	1.12921625	-2.39598379	0.67863034

$C_4H_2N_2(SCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40183443
N	1.12684037	0.00000000	2.10521444
C	2.27169174	0.00000000	1.42208127
C	2.27169174	0.00000000	0.02024684
N	1.14485137	0.00000000	-0.68313317
H	-0.93268982	0.00000000	1.96151138
H	3.20438155	0.00000000	-0.53943011
S	-1.54723902	0.00000000	-0.85484512
S	3.81893076	0.00000000	2.27692639
C	-0.96462899	0.00000000	-2.56915187
H	-0.36937599	0.89088200	-2.77379462
H	-0.36937599	-0.89088200	-2.77379462
H	-1.86249572	0.00000000	-3.19032841
C	3.23632072	0.00000000	3.99123314
H	2.64106772	0.89088200	4.19587589
H	2.64106772	-0.89088200	4.19587589
H	4.13418745	0.00000000	4.61240968
Na	1.13584587	2.40000000	0.71104063

$C_4H_2N_2(SH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40080881
N	1.13014923	0.00000000	2.09886568
C	2.27055951	0.00000000	1.41147125
C	2.27055951	0.00000000	0.01066244
N	1.14041028	0.00000000	-0.68739443
H	-0.92911998	0.00000000	1.96546835
H	3.19967949	0.00000000	-0.55399710
S	-1.53738404	0.00000000	-0.87753287
S	3.80794355	0.00000000	2.28900412
H	-0.94765044	0.00000000	-2.08342742
H	3.21820995	0.00000000	3.49489867
Na	1.13527975	2.45000000	0.70573563

$C_4H_2N_2(CCH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40469782
N	1.12034115	0.00000000	2.11396557
C	2.26575789	0.00000000	1.41887269
C	2.26575789	0.00000000	0.01417487
N	1.14541674	0.00000000	-0.69509287
H	-0.93810577	0.00000000	1.95358816
H	3.20386366	0.00000000	-0.53471547
C	-1.24321709	0.00000000	-0.71878734
C	-2.30245396	0.00000000	-1.29623029
H	-3.23526385	0.00000000	-1.81724365
C	3.50897497	0.00000000	2.13766003
C	4.56821185	0.00000000	2.71510298
H	5.50102173	0.00000000	3.23611634
Na	1.13287895	-2.45000000	0.70943635

$C_4H_2N_2(SiH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40223948
N	1.16297199	0.00000000	2.07627914
C	2.28055010	0.00000000	1.35168929
C	2.28055010	0.00000000	-0.05055019
N	1.11757811	0.00000000	-0.72458985
H	-0.93615786	0.00000000	-0.55520342
H	3.21670796	0.00000000	1.90689271
Si	3.85183079	0.00000000	-1.10240147
H	3.87284444	-1.21023100	-1.95174427
H	3.87284444	1.21023100	-1.95174427
H	5.02364989	0.00000000	-0.19431268
Si	-1.57128069	0.00000000	2.45409076
H	-1.59229434	-1.21023100	3.30343357
H	-1.59229434	1.21023100	3.30343357
H	-2.74309978	0.00000000	1.54600197
Na	1.14027505	-2.45000000	0.67584464

$C_4H_2N_2F_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39302292
N	1.15521343	0.00000000	2.05555314
C	2.24230091	0.00000000	1.32168542
C	2.24230091	0.00000000	-0.07133750
N	1.08708748	0.00000000	-0.73386772
H	-0.92546927	0.00000000	1.95979327
H	3.16777019	0.00000000	-0.63810785
F	-1.16828327	0.00000000	-0.64366282
F	3.41058418	0.00000000	1.96534825
Na	1.12115046	-2.65000000	0.66084271

$C_4H_2N_2(COOCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39928633
N	1.13362950	0.00000000	2.09500053
C	2.25891964	0.00000000	1.38269440
C	2.25891964	0.00000000	-0.01659193
N	1.12529014	0.00000000	-0.71230614
H	-0.93588569	0.00000000	1.94965315
H	3.19480533	0.00000000	-0.56695876
C	-1.32693999	0.00000000	-0.70767102
O	-2.37849962	0.00000000	-0.10914992
O	-1.21252700	0.00000000	-2.03047609
C	3.58585963	0.00000000	2.09036541
O	4.63741926	0.00000000	1.49184432
O	3.47144664	0.00000000	3.41317049

C	-2.45081658	0.00000000	-2.74611456
H	-3.03041772	-0.89068100	-2.49380622
H	-3.03041772	0.89068100	-2.49380622
H	-2.17717433	0.00000000	-3.79951311
C	4.70973622	0.00000000	4.12880895
H	5.28933736	-0.89068100	3.87650062
H	5.28933736	0.89068100	3.87650062
H	4.43609397	0.00000000	5.18220751
Na	1.12945982	-2.55000000	0.69134720

$C_4H_2N_2(COOH)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39640493
N	1.12440156	0.00000000	2.11195866
C	2.27254157	0.00000000	1.43869475
C	2.27254157	0.00000000	0.04228982
N	1.14814001	0.00000000	-0.67326392
H	-0.93180725	0.00000000	-0.55679816
H	3.20434883	0.00000000	1.99549291
C	3.57553818	0.00000000	-0.72036646
O	4.63965794	0.00000000	-0.16200106
O	3.44084060	-0.00000000	-2.04599759
H	2.48908048	-0.00000000	-2.26888747
C	-1.30299661	0.00000000	2.15906121
O	-2.36711636	0.00000000	1.60069581
O	-1.16829903	-0.00000000	3.48469233
H	-0.21653891	-0.00000000	3.70758222
Na	1.13627078	-2.75000000	0.71934738

$C_4H_2N_2(COCH_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39942656
N	1.13466039	0.00000000	2.09438722
C	2.26736111	0.00000000	1.38703242
C	2.26736111	0.00000000	-0.01239414
N	1.13270072	0.00000000	-0.70735480
H	-0.93702067	0.00000000	1.94826332
H	3.20438178	0.00000000	-0.56123090
C	-1.30738694	0.00000000	-0.75374196
O	-2.34926839	0.00000000	-0.13295416
C	3.57474805	0.00000000	2.14077438
O	4.61662950	0.00000000	1.51998658
C	-1.24291171	0.00000000	-2.25740700
H	-0.69297654	0.87701900	-2.61109927
H	-0.69297654	-0.87701900	-2.61109927
H	-2.25894058	0.00000000	-2.65358695
C	3.51027282	0.00000000	3.64443942
H	2.96033765	0.87701900	3.99813169
H	2.96033765	-0.87701900	3.99813169
H	4.52630169	0.00000000	4.04061937
Na	1.13368056	2.55000000	0.69351621

$C_4H_2N_2(OCF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39830899
N	1.15231924	0.00000000	2.05906139
C	2.26331201	0.00000000	1.35400743
C	2.26331201	0.00000000	-0.04430156
N	1.11099278	0.00000000	-0.70505396
H	-0.90756525	0.00000000	1.99135918
H	3.17087727	0.00000000	-0.63735175
O	-1.13218505	0.00000000	-0.78742724
O	3.39549707	0.00000000	2.14143467
C	-2.35888690	0.00000000	-0.21720174
C	4.62219891	0.00000000	1.57120917
F	-3.25431744	0.00000000	-1.18824552
F	-2.55944031	-1.07859900	0.55264221
F	-2.55944031	1.07859900	0.55264221
F	4.82275233	1.07859900	0.80136522
F	5.51762946	0.00000000	2.54225295
F	4.82275233	-1.07859900	0.80136522
Na	1.13165600	-2.65000000	0.67700372

$C_4H_2N_2(BF_2)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40333184
N	1.15033357	0.00000000	2.09651426
C	2.27051316	0.00050714	1.37910476
C	2.27051298	0.00104714	-0.02422697
N	1.12017958	0.00053114	-0.71740950
H	-0.93739344	0.00000724	-0.55178932
H	3.20790646	0.00093990	1.93089416
B	-1.34405098	-0.00041802	2.21280915
B	3.61456383	0.00185516	-0.83370421
F	-2.49881013	-0.00046363	1.56174946
F	4.76932282	0.00234477	-0.18264443
F	-1.36401530	-0.00092582	3.52781117
F	3.63452831	0.00186695	-2.14870633
Na	1.13614106	-2.59945823	0.68905220

$C_4H_2N_2(CHO)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39985756
N	1.12517921	0.00000000	2.11847751
C	2.26247295	0.00000000	1.42895845
C	2.26247295	0.00000000	0.02910089
N	1.13729374	0.00000000	-0.68951906
H	-0.93600776	0.00000000	-0.55135405
H	3.19848070	0.00000000	1.98031250
C	-1.28037766	0.00000000	2.17257429
O	-2.36464802	0.00000000	1.64290619
H	-1.15410409	0.00000000	3.27077962
C	3.54285061	0.00000000	-0.74361584
O	4.62712097	0.00000000	-0.21394774
H	3.41657704	0.00000000	-1.84182117
Na	1.13123648	-2.60000000	0.71447923

$C_4H_2N_2(CF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39561450
N	1.11365916	0.00000000	2.11684309
C	2.25861689	0.00000000	1.43901882
C	2.25861689	0.00000000	0.04340432
N	1.14495773	0.00000000	-0.67782427

H	-0.92253248	0.00000000	-0.57156197
H	3.18114937	0.00000000	2.01058079
C	-1.28888693	0.00000000	2.19088385
C	3.54750382	0.00000000	-0.75186503
F	-2.35530687	0.00000000	1.37508878
F	-1.37369883	1.08053100	2.97329155
F	-1.37369883	-1.08053100	2.97329155
F	3.63231571	-1.08053100	-1.53427273
F	3.63231571	1.08053100	-1.53427273
F	4.61392375	0.00000000	0.06393004
Na	1.12930844	2.70000000	0.71950941

$C_4H_2N_2(NO)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39905447
N	1.10539132	0.00000000	2.13170834
C	2.25299462	0.00000000	1.45966477
C	2.25299462	0.00000000	0.06061030
N	1.14760329	0.00000000	-0.67204357
H	-0.92601210	0.00000000	-0.56576244
H	3.17900672	0.00000000	2.02542721
N	-1.23224107	0.00000000	2.19804405
O	-2.22603402	0.00000000	1.52475682
N	3.48523569	0.00000000	-0.73837927
O	4.47902864	0.00000000	-0.06509205
Na	1.12649731	-2.70000000	0.72983239

$C_4H_2N_2(SiF_3)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40155571
N	1.14625747	0.00000000	2.09954078
C	2.27527615	0.00000000	1.39435667
C	2.27527615	0.00000000	-0.00719904
N	1.12901868	0.00000000	-0.70518411
H	-0.93070274	0.00000000	-0.56260759
H	3.20597889	0.00000000	1.95696426
Si	3.82695559	0.00000000	-1.02633234
Si	-1.55167944	0.00000000	2.42068901
F	5.07950756	0.00000000	-0.04339050
F	3.91765042	-1.28409900	-1.95447147
F	3.91765042	1.28409900	-1.95447147
F	-1.64237427	-1.28409900	3.34882814
F	-1.64237427	1.28409900	3.34882814
F	-2.80423141	0.00000000	1.43774717
Na	1.13763808	-2.65000000	0.69717834

$C_4H_2N_2(CN)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40192850
N	1.12476213	0.00000000	2.11954550
C	2.25817632	0.00000000	1.42952436
C	2.25817632	0.00000000	0.02759586
N	1.13341420	0.00000000	-0.69002114
H	-0.93071202	0.00000000	-0.56037108
H	3.18888834	0.00000000	1.98989544
C	-1.25852475	0.00000000	2.11411784
N	-2.28421052	0.00000000	2.64704173
C	3.51670107	0.00000000	-0.68459349
N	4.54238685	0.00000000	-1.21751737
Na	1.12908816	-2.80000000	0.71476218

$C_4H_2N_2Cl_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39753159
N	1.14397003	0.00000000	2.07555168
C	2.25546679	0.00000000	1.36407621
C	2.25546679	0.00000000	-0.03345538
N	1.11149676	0.00000000	-0.71147547
H	-0.92598710	0.00000000	1.96438921
H	3.18145389	0.00000000	-0.60031299
Cl	3.76442166	0.00000000	2.21712923
Cl	-1.50895487	0.00000000	-0.85305302
Na	1.12773340	-2.60000000	0.68203811

$C_4H_2N_2Br_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39685828
N	1.14198934	0.00000000	2.07754534
C	2.25450325	0.00000000	1.36744237
C	2.25450325	0.00000000	-0.02941591
N	1.11251391	0.00000000	-0.71010296
H	-0.92641711	0.00000000	1.96310743
H	3.18092036	0.00000000	-0.59566506
Br	3.88779627	0.00000000	2.29097777
Br	-1.63329302	0.00000000	-0.92353540
Na	1.12725163	-2.60000000	0.68372119

$C_4H_2N_2(NC)_2\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40059076
N	1.13638969	0.00000000	2.08434927
C	2.25361457	0.00000000	1.36654993
C	2.25361457	0.00000000	-0.03404083
N	1.11722488	0.00000000	-0.71779934
H	-0.93157361	0.00000000	1.95896680
H	3.18518818	0.00000000	-0.59241686
N	3.45716953	0.00000000	2.04436797
N	-1.20355496	0.00000000	-0.67781803
C	4.49220392	0.00000000	2.60264508
C	-2.23858934	0.00000000	-1.23609514
Na	1.12680729	-2.70000000	0.68327496

$C_4N_2X_4\cdots Na^+$ geometries

$C_4N_2(OH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39970400
N	1.14110900	0.00000000	2.07046500
C	2.28221800	0.00000000	1.39970400
C	2.28221800	0.00000000	-0.00000000
N	1.14110900	0.00000000	-0.67076100
O	-1.17371400	0.00000000	2.06354600
H	-0.97253400	0.00000000	3.01325100

O	3.45593200	0.00000000	-0.66384200
H	3.25475200	0.00000000	-1.61354700
O	-1.17371400	0.00000000	-0.66384200
H	-0.97253400	0.00000000	-1.61354700
O	3.45593200	0.00000000	2.06354600
H	3.25475200	0.00000000	3.01325100
Na	1.14110900	-2.45000000	0.69985200

$C_4N_2(CH_3)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40535400
N	1.14615500	0.00000000	2.08882100
C	2.29230999	0.00000000	1.40535400
C	2.29230999	0.00000000	0.00000000
N	1.14615500	0.00000000	-0.68346700
C	3.57512099	0.00000000	-0.78440700
H	4.18337099	0.88191600	-0.55197800
H	4.18337099	-0.88191600	-0.55197800
H	3.34613699	0.00000000	-1.85132799
C	3.57512099	0.00000000	2.18976100
H	4.18337099	-0.88191600	1.95733200
H	4.18337099	0.88191600	1.95733200
H	3.34613699	0.00000000	3.25668199
C	-1.28281100	0.00000000	-0.78440700
H	-1.89106100	-0.88191600	-0.55197800
H	-1.89106100	0.88191600	-0.55197800
H	-1.05382700	0.00000000	-1.85132799
C	-1.28281100	0.00000000	2.18976100
H	-1.89106100	0.88191600	1.95733200
H	-1.89106100	-0.88191600	1.95733200
H	-1.05382700	0.00000000	3.25668199
Na	1.14615499	2.35000000	0.70267700

$C_4N_2(NH_2)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40524219
N	1.13912000	0.00000000	2.08829334
C	2.27639111	-0.04555572	1.40368224
C	2.27259593	-0.13906675	0.00155995
N	1.13537352	-0.09231123	-0.68305115
N	-1.21790418	0.08533822	2.09197503
H	-1.91927398	-0.55507057	1.72791118
H	-1.08646929	-0.04854466	3.08925619
N	-1.22081416	0.01363814	-0.68673284
H	-1.86798018	0.70877780	-0.32266899
H	-1.07896203	0.13642955	-1.68401400
N	3.49615320	-0.08511611	2.09127995
H	4.19647959	0.52958368	1.68351455
H	3.36740013	0.11484534	3.07779277
N	3.49155217	-0.19848272	-0.68603776
H	4.13976161	-0.86791338	-0.27827236
H	3.34701823	-0.38735270	-1.67255058
Na	1.23249109	2.30060769	0.62432356

$C_4N_2(SH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40817400
N	1.14304200	0.00000000	2.08342600
C	2.28608401	0.00000000	1.40817400
C	2.28608401	0.00000000	-0.00000000
N	1.14304200	0.00000000	-0.67525200
S	-1.52599500	0.00000000	2.29995800
H	-0.91968000	-0.00000000	3.49656300
S	3.81207901	0.00000000	-0.89178400
H	3.20576401	-0.00000000	-2.08838900
S	-1.52599500	0.00000000	-0.89178400
H	-0.91968000	0.00000000	-2.08838900
S	3.81207901	0.00000000	2.29995800
H	3.20576401	0.00000000	3.49656300
Na	1.14304201	-2.40000000	0.70408700

$C_4N_2(CCH)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41675800
N	1.14049600	0.00000000	2.10730500
C	2.28099200	0.00000000	1.41675800
C	2.28099200	0.00000000	-0.00000000
N	1.14049600	0.00000000	-0.69054700
C	-1.22987100	0.00000000	2.15525300
C	-2.26644600	0.00000000	2.77139200
H	-3.18227300	0.00000000	3.32204600
C	-1.22987100	0.00000000	-0.73849500
C	-2.26644600	0.00000000	-1.35463400
H	-3.18227300	0.00000000	-1.90528800
C	3.51086300	0.00000000	-0.73849500
C	4.54743800	0.00000000	-1.35463400
H	5.46326500	0.00000000	-1.90528800
C	3.51086300	0.00000000	2.15525300
C	4.54743800	0.00000000	2.77139200
H	5.46326500	0.00000000	3.32204600
Na	1.14049600	-2.50000000	0.70837900

$C_4N_2F_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39607400
N	1.11833900	0.00000000	2.07957100
C	2.23667800	0.00000000	1.39607400
C	2.23667800	0.00000000	-0.00000000
N	1.11833900	0.00000000	-0.68349700
F	-1.14635700	0.00000000	2.05635500
F	-1.14635700	0.00000000	-0.66028100
F	3.38303500	0.00000000	2.05635500
F	3.38303500	0.00000000	-0.66028100
Na	1.11833900	-3.00000000	0.69803700

$C_4N_2(CN)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41084000
N	1.13301800	0.00000000	2.10532200
C	2.26603600	0.00000000	1.41084000
C	2.26603600	0.00000000	0.00000000
N	1.13301800	0.00000000	-0.69448200
C	-1.24024500	0.00000000	-0.73744900
N	-2.24453799	0.00000000	-1.30871100

C	-1.24024500	0.00000000	2.14828900
N	-2.24453799	0.00000000	2.71955100
C	3.50628100	0.00000000	2.14828900
N	4.51057400	0.00000000	2.71955100
C	3.50628100	0.00000000	-0.73744900
N	4.51057400	0.00000000	-1.30871100
Na	1.13301800	-2.85000000	0.70542000

$C_4N_2Cl_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40555000
N	1.13587900	0.00000000	2.07407200
C	2.27175800	0.00000000	1.40555000
C	2.27175800	0.00000000	0.00000000
N	1.13587900	0.00000000	-0.66852200
Cl	3.73234000	0.00000000	-0.90910200
Cl	3.73234000	0.00000000	2.31465200
Cl	-1.46058200	0.00000000	-0.90910200
Cl	-1.46058200	0.00000000	2.31465200
Na	1.13587900	-2.65000000	0.70277500

$C_4N_2Br_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40367600
N	1.13711000	0.00000000	2.06909700
C	2.27421999	0.00000000	1.40367600
C	2.27421999	0.00000000	0.00000000
N	1.13711000	0.00000000	-0.66542100
Br	-1.57103700	0.00000000	2.41512400
Br	3.84525700	0.00000000	-1.01144800
Br	-1.57103700	0.00000000	-1.01144800
Br	3.84525700	0.00000000	2.41512400
Na	1.13710999	-2.60000000	0.70183800

$C_4N_2(NC)_4\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41145000
N	1.12936500	0.00000000	2.10003000
C	2.25873000	0.00000000	1.41145000
C	2.25873000	0.00000000	0.00000000
N	1.12936500	0.00000000	-0.68858000
N	-1.18680800	0.00000000	2.09803800
N	3.44553800	0.00000000	-0.68658800
C	-2.22354600	0.00000000	2.65812600
C	4.48227600	0.00000000	-1.24667600
N	-1.18680800	0.00000000	-0.68658800
N	3.44553800	0.00000000	2.09803800
C	-2.22354600	0.00000000	-1.24667600
C	4.48227600	0.00000000	2.65812600
Na	1.12936500	-2.70000000	0.70572500

$C_3N_3X_3\cdots Na^+$ geometries

$C_3N_3H_3\cdots Na^+$

C	0.00000000	1.29199700	0.00000000
N	1.18603000	0.68475500	0.00000000
C	1.11890200	-0.64599800	0.00000000
N	0.00000000	-1.36950900	0.00000000
C	-1.11890200	-0.64599800	0.00000000
N	-1.18603000	0.68475500	0.00000000
H	2.06069900	-1.18974500	0.00000000
H	0.00000000	2.37949000	0.00000000
H	-2.06069900	-1.18974500	0.00000000
Na	0.00000000	0.00000000	2.65000000

$C_3N_3(CH_2OH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.34141340
C	1.19717960	0.00000000	1.90825225
N	2.35887796	0.00000000	1.23754504
C	2.25118473	0.00000000	-0.08266199
N	1.08948638	0.00000000	-0.75336818
C	1.26201087	0.00000000	3.41263271
C	-1.33524709	0.00000000	-0.69604461
C	3.52160056	0.00000000	-0.89099784
O	0.00119418	0.00000000	4.01799634
O	-1.22909877	0.00000000	-2.09062658
O	4.67627027	0.00000000	-0.10177992
H	1.83572150	0.88407300	3.72310995
H	1.83572150	-0.88407300	3.72310995
H	-1.89098409	0.88407300	-0.35443600
H	-1.89098409	-0.88407300	-0.35443600
H	3.50362692	0.88407300	-1.54308370
H	3.50362692	-0.88407300	-1.54308370
H	-0.67329049	0.00000000	3.31790407
H	-0.28555887	0.00000000	-2.32470041
H	4.40721370	0.00000000	0.83238660
Na	1.14945478	2.65000000	0.60853009

$C_3N_3(NHOH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.34111621
C	1.22050798	0.00000000	1.86083475
N	2.38194779	-0.00018050	1.19027750
C	2.22178335	-0.00016769	-0.12657256
N	1.06034270	-0.00017919	-0.79713095
N	1.34880571	0.08510900	3.23000854
N	-1.24988196	0.08511657	-0.57348809
N	3.34338671	0.08476573	-0.92226960
O	0.29892314	-0.42927975	3.98147280
O	-1.37576336	-0.42943659	-1.85837676
O	4.51903726	-0.42979535	-0.38877320
H	2.23203743	-0.26605437	3.58386278
H	-1.99796950	-0.26591694	0.01453241
H	3.20816477	-0.26638538	-1.86409573
H	-0.26606799	0.33506042	4.17129817
H	-1.25760966	0.33481693	-2.44268852
H	4.96604208	0.33448095	0.00560461
Na	1.14715565	-2.45008788	0.57827093

$C_3N_3(N(CH_3)_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.34164943

C	1.22119941	0.00000000	1.89529702
N	2.38278083	0.03024779	1.22459946
C	2.25179998	0.02857883	-0.10982727
N	1.08982514	0.03023560	-0.78052565
C	3.35451568	0.25896621	-2.27561453
H	4.20845918	-0.23896547	-2.74349313
H	2.42988002	-0.14337926	-2.68481025
H	3.40383193	1.33344571	-2.50615774
C	4.67647016	0.23965588	-0.19250407
H	4.70036727	-0.28286147	0.76256863
H	5.46782532	-0.14754024	-0.83972548
H	4.86034907	1.30855938	-0.01018387
N	3.40010199	0.01995317	-0.84575291
N	1.28477849	-0.03860530	3.25718137
N	-1.21082677	-0.03852087	-0.62663805
C	-1.28870892	0.18104852	-2.05836527
H	-0.46053303	-0.32004550	-2.55715300
H	-2.23475887	-0.22978505	-2.42067040
H	-1.24981920	1.25158824	-2.30744143
C	-2.43204911	0.16870706	0.12793472
H	-3.25130309	-0.34950844	-0.37836738
H	-2.31403070	-0.23201999	1.13280537
H	-2.68350135	1.23707218	0.20179904
C	0.07857331	0.14951740	4.04063344
H	-0.18361398	1.21364700	4.13278808
H	-0.75448340	-0.37225769	3.57209686
H	0.24810643	-0.25838971	5.04059799
C	2.54316449	0.19971941	3.93789719
H	2.52737667	-0.32025085	4.89989893
H	3.36433134	-0.17959140	3.33284870
H	2.70573518	1.27232033	4.12006805
Na	1.18590227	-2.28516190	0.57696336

$C_3N_3(NHCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33388701
C	1.23608146	0.00000000	1.87434003
N	2.39120452	-0.00021739	1.20736124
C	2.24132253	-0.00018752	-0.13337439
N	1.08613366	-0.00011162	-0.80022242
N	1.29480725	0.00023783	3.22484585
C	2.53982512	-0.00225887	3.96008865
N	-1.19878188	0.00005830	-0.62467218
C	-2.45833117	-0.00161777	0.08533667
N	3.38170950	-0.00050053	-0.85927842
C	3.39679084	0.00045568	-2.30515067
H	0.40774502	-0.00138509	3.70521499
H	3.13848178	0.88189794	3.71945177
H	2.30944102	-0.00013342	5.02680358
H	3.13400613	-0.89018613	3.72194852
H	-1.17070977	-0.00129544	-1.63306660
H	-2.54972320	0.88296222	0.72344312
H	-3.26639703	0.00031057	-0.64816661
H	-2.55015968	-0.88915732	0.71936088
H	4.24100190	0.00055865	-0.33084473
H	2.89194025	0.88681045	-2.70211786
H	4.43603986	0.00061873	-2.63804517
H	2.89198317	-0.88545721	-2.70311161
Na	1.15879062	-2.30008573	0.58050435

$C_3N_3(OCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33971821
C	1.21461912	0.00000000	1.86582389
N	2.37484892	0.00000000	1.19596558
C	2.22316055	0.00000000	-0.11897843
N	1.06293074	0.00000000	-0.78883834
O	1.34885279	0.00000000	3.18564688
O	-1.21011681	0.00000000	-0.54366057
O	3.29904310	0.00000000	-0.89514003
C	4.57176862	0.00000000	-0.24770222
C	-1.28578114	0.00000000	-1.96959276
C	0.15179276	0.00000000	3.96413962
H	4.68317081	-0.88991600	0.37577554
H	4.68317081	0.88991600	0.37577554
H	5.30056713	0.00000000	-1.05679511
H	-2.35087620	0.00000000	-2.19620415
H	-0.80153565	-0.88991600	-2.37780847
H	-0.80153565	0.88991600	-2.37780847
H	-0.44385550	-0.88991600	3.74887840
H	-0.44385550	0.88991600	3.74887840
H	0.48808793	0.00000000	4.99984415
Na	1.14592656	-2.45000000	0.58228182

$C_3N_3(OH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32895352
C	1.22303849	0.00000000	1.85457283
N	2.37394564	0.00000000	1.19009548
C	2.21762553	0.00000000	-0.13189619
N	1.06671839	0.00000000	-0.79637236
O	1.31879401	0.00000000	3.17958503
O	-1.19537268	-0.00000000	-0.57957932
O	3.31724268	0.00000000	-0.87732908
H	0.41449492	0.00000000	3.53748409
H	-1.05317260	-0.00000000	-1.54167458
H	4.07934171	0.00000000	-0.27313287
Na	1.14688801	-2.60000000	0.57422554

$C_3N_3(CH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33652986
C	1.20727146	0.00000000	1.90994741
N	2.36435216	0.00249280	1.24130339
C	2.25788197	0.00168102	-0.09066989
N	1.10040582	0.00249280	-0.75830576
C	3.52453017	-0.02568602	-0.89131404
C	-1.32565706	-0.02762826	-0.69853761
C	1.26949940	-0.02762826	3.40709440
H	3.81095188	-1.06808492	-1.07236026
H	3.37238584	0.45608152	-1.85847346
H	4.33287854	0.45608152	-0.33893902
H	-2.10123758	0.39246250	-0.05654566
H	-1.26709289	0.51533360	-1.64359433

H	-1.59115687	-1.06691790	-0.92379477
H	0.35684486	0.39246250	3.83223027
H	1.35906289	-1.06691790	3.74356033
H	2.14828390	0.51533360	3.75965612
X	1.15498551	0.00111161	0.60646733
Na	1.15100688	2.45110735	0.60871628

$C_3N_3(NH_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33875191
C	1.22631059	0.00000000	1.87607803
N	2.38598315	-0.00801184	1.20689167
C	2.23788388	-0.00720669	-0.12381528
N	1.07839845	-0.00768277	-0.79325559
N	1.30131216	0.03037119	3.22939594
N	-1.20934784	0.02983351	-0.61181213
N	3.37254627	0.01561522	-0.86546035
H	0.45743208	-0.12633173	3.75865850
H	2.19735288	-0.13243492	3.66226164
H	-1.24619251	-0.13168071	-1.60646984
H	-2.03287103	-0.12607622	-0.05119635
H	4.25171076	-0.14707066	-0.39923014
H	3.29838094	-0.14657132	-1.85793366
Na	1.16661364	2.34614129	0.57651043

$C_3N_3(SCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.34365241
C	1.21084765	0.00000000	1.88501618
N	2.37448522	0.00000000	1.21318960
C	2.23789649	0.00000000	-0.10611690
N	1.07425893	0.00000000	-0.77794272
C	4.96928096	0.00000000	0.12696214
C	-1.16384043	0.00000000	-2.48198877
C	-0.35669638	0.00000000	4.13392592
S	1.38315137	0.00000000	3.62909335
S	-1.59656639	0.00000000	-0.72281925
S	3.66215917	0.00000000	-1.12737481
H	4.90336457	-0.89051100	0.75279341
H	4.90336457	0.89051100	0.75279341
H	5.91204540	0.00000000	-0.42388472
H	-2.11226977	0.00000000	-3.02302278
H	-0.58889586	-0.89051100	-2.73781872
H	-0.58889586	0.89051100	-2.73781872
H	-0.86572368	-0.89051100	3.76392414
H	-0.86572368	0.89051100	3.76392414
H	-0.35103148	0.00000000	5.22580679
Na	1.14958138	-2.40000000	0.59296643

$C_3N_3(SH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33511237
C	1.21757419	0.00000000	1.87599454
N	2.37381614	0.00000000	1.20843918
C	2.23344593	0.00000000	-0.11645282
N	1.07720485	0.00000000	-0.78400936
S	-1.58850550	0.00000000	-0.74549499
S	1.36620963	0.00000000	3.62442816
S	3.67331598	0.00000000	-1.11939146
H	-1.10320843	0.00000000	-1.99730102
H	0.03946572	0.00000000	3.83005144
H	4.51476419	0.00000000	-0.07320912
Na	1.15034034	-2.50000000	0.58651406

$C_3N_3(CCH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33636287
C	1.21720182	0.00000000	1.88818183
N	2.37466472	0.00000000	1.22002149
C	2.24381488	0.00000000	-0.11002884
N	1.08639647	0.00000000	-0.77821075
C	1.28923406	0.00000000	3.32783761
C	-1.28214555	-0.00000000	-0.65872262
C	3.45612921	0.00000000	-0.88983231
C	4.47045124	0.00000000	-1.53947491
C	-2.35350808	-0.00000000	-1.20915305
C	1.35178041	0.00000000	4.53073937
H	5.37166622	0.00000000	-2.11415422
H	-3.30417014	-0.00000000	-1.69757047
H	1.40940174	0.00000000	5.59803801
Na	1.15367950	-2.60000000	0.59272102

$C_3N_3(SiH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.34117475
C	1.20536365	0.00000000	1.92926333
N	2.36685394	0.00177602	1.25867638
C	2.27347226	0.00170595	-0.07924348
N	1.11198061	0.00177602	-0.74983043
Si	-1.68214911	-0.04946123	-0.89459608
Si	1.27176880	-0.04946123	3.83334267
Si	3.88932337	-0.04528055	-1.08879369
H	-2.69044955	0.62116569	-0.04852888
H	-2.04929841	-1.46991726	-1.09104975
H	-1.54486569	0.62299538	-2.20272272
H	0.06924942	0.62116569	4.36854976
H	1.28733859	-1.46991726	4.24945592
H	2.50762797	0.62299538	4.28355835
H	4.95307936	0.62690118	-0.31494949
H	4.24403194	-1.46519492	-1.31040823
H	3.66028467	0.62690118	-2.38415192
Na	1.16144769	-2.49913089	0.61552636

$C_3N_3(COOCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32822333
C	1.21365047	0.00000000	1.87562998
N	2.36392435	0.00106156	1.21151819
C	2.23116718	0.00100281	-0.11323742
N	1.08089197	0.00106325	-0.77734809
C	-1.33690983	-0.02256941	-0.72579731
O	-1.44245426	-0.30619060	-1.88985895
C	1.25356577	-0.02260283	3.39632478
O	0.29848627	-0.30711111	4.06974725

C	3.52818984	-0.02040094	-0.90815312
O	4.58918525	-0.30398036	-0.41775430
O	3.32793590	0.30573701	-2.17974203
O	-2.33830224	0.30263400	0.08343627
O	2.45478700	0.30365668	3.85895401
C	4.50108918	0.29215527	-2.99921159
C	2.57789832	0.28898580	5.28465834
C	-3.63454760	0.28791762	-0.52280976
H	5.23065557	1.01156736	-2.62104337
H	4.16210059	0.56787439	-3.99572546
H	4.94438486	-0.70608073	-2.99999825
H	3.61028523	0.56496340	5.48956250
H	2.35734001	-0.70964729	5.66815851
H	1.88531748	1.00776068	5.72797192
H	-4.32830624	0.56297879	0.26903191
H	-3.85598207	-0.71049987	-0.90636752
H	-3.67247207	1.00733336	-1.34368403
Na	1.14944763	-2.69996937	0.58670384

$C_3N_3(COOH)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33139939
C	1.21052807	0.00000000	1.87642317
N	2.36355388	0.00000000	1.21072328
C	2.23029416	0.00000000	-0.11013659
N	1.07726880	0.00000000	-0.77583697
C	1.32234112	0.00000000	3.39336380
C	-1.36961521	0.00000000	-0.66163768
C	3.48809632	0.00000000	-0.96543954
O	3.46403896	0.00000000	-2.16545033
O	-2.39682687	0.00000000	-0.04079734
O	2.37361013	0.00000000	3.97253426
O	-1.27747016	0.00000000	-1.99291055
O	0.12335192	0.00000000	3.97920100
O	4.59494089	0.00000000	-0.22000253
H	-2.18429219	0.00000000	-2.34710755
H	0.27001979	0.00000000	4.94162989
H	5.35509462	0.00000000	-0.82823577
Na	1.14694075	-2.90000000	0.58876219

$C_3N_3(COCH_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32845753
C	1.21179595	0.00000000	1.88969784
N	2.36227388	0.00000000	1.22546818
C	2.24242454	0.00000000	-0.10459751
N	1.09194566	0.00000000	-0.76882569
C	-1.36035589	-0.00000000	-0.70147407
O	-1.39893369	-0.00000000	-1.90688110
C	1.28447966	0.00000000	3.41853767
O	0.25985577	0.00000000	4.05464985
C	3.53009578	0.00000000	-0.93196359
O	4.59329746	0.00000000	-0.36266874
C	3.37112728	-0.00000000	-2.42748141
C	2.65912004	-0.00000000	4.02862537
C	-2.57602777	-0.00000000	0.18395604
H	2.79757987	-0.87544600	-2.74743536
H	2.79757987	0.87544600	-2.74743536
H	4.35956552	0.00000000	-2.88704292
H	3.22298269	-0.87544600	3.69189520
H	3.22298269	0.87544600	3.69189520
H	2.56289454	0.00000000	5.11441824
H	-2.56634269	-0.87544600	0.84063923
H	-2.56634269	0.87544600	0.84063923
H	-3.46823957	-0.00000000	-0.44227499
Na	1.15140651	-2.65000000	0.59503333

$C_3N_3(OCF_3)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32834186
C	1.21568606	0.00000000	1.83854192
N	2.36606420	0.00000000	1.17437037
C	2.20006699	0.00000000	-0.13354478
N	1.04968885	0.00000000	-0.79771509
O	1.37831256	0.00000000	3.17737457
O	-1.24077751	0.00000000	-0.52857814
O	3.27821737	0.00000000	-0.94380006
C	4.54844214	0.00000000	-0.40699154
C	-1.41100027	0.00000000	-1.89702874
C	0.27831040	0.00000000	4.00901805
F	-0.47065944	-1.08151800	3.83536946
F	4.77254311	-1.08151800	0.32845923
F	-0.88613063	-1.08151800	-2.45883155
F	-0.88613063	1.08151800	-2.45883155
F	-2.71763737	0.00000000	-2.10202261
F	5.37929108	0.00000000	-1.43607670
F	0.75410012	0.00000000	5.24309583
F	-0.47065944	1.08151800	3.83536946
F	4.77254311	1.08151800	0.32845923
Na	1.13858435	-3.05000000	0.56833238

$C_3N_3(BF_2)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33895928
C	1.20671282	0.00000000	1.91918070
N	2.36628565	0.00000000	1.24970150
C	2.26541569	0.00000000	-0.08545272
N	1.10584286	0.00000000	-0.75493280
B	1.26662036	0.00000000	3.50736944
B	-1.40536543	-0.00000000	-0.74221271
B	3.61087358	0.00000000	-0.93142874
F	0.15709358	0.00000000	4.21179384
F	2.42606221	0.00000000	4.12620681
F	-1.46065106	-0.00000000	-2.05530330
F	3.56708176	0.00000000	-2.24495289
F	4.77568688	0.00000000	-0.32276209
F	-2.52101458	-0.00000000	-0.04752547
Na	1.15737646	-2.75000000	0.61124282

$C_3N_3(CHO)_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33586952
C	1.20892355	0.00000000	1.88546641
N	2.36564021	0.00000000	1.21749974

C	2.23733557	0.00000000	-0.10407121
N	1.08058706	0.00000000	-0.77207609
C	1.24232803	0.00000000	3.40036387
C	-1.32796310	0.00000000	-0.73000542
C	3.53277559	0.00000000	-0.89019759
O	3.56095809	0.00000000	-2.08991200
O	-2.38179778	0.00000000	-0.15625908
O	2.26746377	0.00000000	4.02414693
H	0.24294091	0.00000000	3.87020044
H	-1.23309742	0.00000000	-1.83008386
H	4.43901001	0.00000000	-0.25951124
Na	1.14874760	-2.95000000	0.59378120

$C_3N_3Cl_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32618239
C	1.21830458	0.00000000	1.85020727
N	2.36641636	0.00000000	1.18662559
C	2.21145553	0.00000000	-0.13037419
N	1.06278059	0.00000000	-0.79325730
Cl	3.64888459	0.00000000	-1.07230673
Cl	-1.53615254	0.00000000	-0.77029468
Cl	1.32325505	0.00000000	3.56555697
Na	1.14438566	-2.75000000	0.57384547

$C_3N_3Br_3\cdots Na^+$

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.32588609
C	1.21827869	0.00000000	1.84911839
N	2.36653034	0.00000000	1.18617510
C	2.21052282	0.00000000	-0.13050151
N	1.06227117	0.00000000	-0.79344431
Br	3.76874859	0.00000000	-1.15712741
Br	-1.66819772	0.00000000	-0.83615011
Br	1.32825064	0.00000000	3.71189440
Na	1.14293384	-2.70000000	0.57287229