Electronic Supplementary Information

for

Substituent effects on the [1-*closo*-CB_9H_{10}]$^-$ anion geometry: Experimental and DFT studies

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1. Structure solution and refinement

Single crystal X-ray diffraction measurements for **1l[PyrCH$_2$Cl]**, **1m[Et$_4$N][Et$_4$NBr]**, **1n**, **1o** and **1q** were performed with a Bruker Nonius Kappa CCD diffractometer. The crystals of **1l[PyrCH$_2$Cl]**, **1m[Et$_4$N][Et$_4$NBr]**, **1n** and **1q** were kept at 150(2) K during data collection, while measurements for **1o** were conducted at 195(2) K. Data collections were performed using the Mo *K*α radiation (λ = 0.71073 Å). The data were integrated using DENZO-SMN[1] and COLLECT program.[2] Intensities for absorption were corrected using multi-scan method as implemented in DENZO-SMN. Additional information is listed in Table S1.

All structures were solved with the ShelXS-97[3] structure solution program using direct method and refined in the ShelXL-97[4] by the full-matrix least-squares minimization on F^2. All non-hydrogen atoms were refined anisotropically. C−H and B–H hydrogens were generated geometrically using the HFIX command in ShelXL.

CCDC: 265347–265351 contain the supplementary crystallographic data for this paper. The data is provided free of charge by The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S1. Crystal data and structure refinement

Identification code	**1l[PyrCH$_2$Cl]**	**1m[Et$_4$N][Et$_4$NBr]**	**1n**	**1o**	**1q**
CCDC:	265347	265348	265349	265350	265351
Formula	$C_7H_{16}B_9Cl_2N$	$C_{46}H_{110}B_{18}Br_2N_{10}$	$C_3H_{15}B_9S$	$C_6H_{14}B_9N$	$CH_8B_9IN_2$
Formula weight	282.4	1157.84	180.5	197.47	272.28
Size /mm	0.50x0.33x0.13	0.66x0.23x0.07	0.30x0.17x0.03	0.59x0.26x0.07	0.20x0.17x0.07
Crystal colour	yellow	yellow	colourless	colourless	yellow
Crystal shape	prism	prism	prism	needle	block
Wavelength	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_1$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	Cc
a /Å	9.9849(2)	9.0602(1)	6.4442(5)	10.1476(4)	16.2967(5)
b /Å	14.3250(3)	16.8803(1)	8.1244(7)	10.8518(5)	6.5799(3)
c /Å	10.8831(2)	22.9672(2)	10.6645(8)	13.7392(6)	11.8991(5)
α /°	90	104.577(5)	85.078(5)	90	90
β /°	102.415(1)	92.623(4)	82.012(5)	130.476(3)	126.545(3)
γ /°	90	90.179(5)	74.701(3)	90	90
Volume /Å^3	1520.25(5)	3395.56(5)	532.62(7)	1150.87(9)	1025.08(7)
Z	4	2	2	4	4
D_{calc} /g cm^{-3}	1.234	1.132	1.125	1.140	1.764
Abs. coefficient /mm^{-1}	0.401	1.232	0.239	0.055	3.061
F(000)	576	1232	188	408	504
θ range for data collection /°	2.51 to 27.49	2.89 to 26	2.6 to 26	3.24 to 26	3.47 to 26
Index ranges	-12 ≤ h ≤12, -18 ≤ k ≤ 17, -13 ≤ l ≤ 14	-11 ≤ h ≤11, -20 ≤ k ≤ 19, -28 ≤ l ≤ 28	-7 ≤ h ≤7, -10 ≤ k ≤ 10, -12 ≤ l ≤ 13	-12 ≤ h ≤12, -13 ≤ k ≤ 13, -16 ≤ l ≤ 16	-20 ≤ h ≤19, -8 ≤ k ≤ 8, -14 ≤ l ≤ 14
No. of measured, independent, and observed [$I>2\sigma(I)$] reflections	17724, 6746, 5817	42246, 13239, 10459	8951, 2065, 1606	9290, 2200, 1843	8689, 1990, 1782
R_{int}	0.0759	0.1058	0.1359	0.1109	0.0776
Abs. correction	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Data / restraints / parameters	6746 / 1 / 471	13239 / 0 / 853	2065 / 0 / 120	2200 / 0 / 159	1990 / 2 / 118
Goodness of fit	1.04	1.02	1.23	1.02	1.08
Final R indices [I >2s(I)]	R_1 = 0.0482, wR_2 = 0.1184	R_1 = 0.0579 wR_2 = 0.1417	R_1 = 0.0995 wR_2 = 0.288	R_1 = 0.0564 wR_2 = 0.1502	R_1 = 0.0345 wR_2 = 0.0834
R indices (all data)	R_1 = 0.0591, wR_2 = 0.125	R_1 = 0.0754, wR_2 = 0.1563	R_1 = 0.1233, wR_2 = 0.3007	R_1 = 0.0662, wR_2 = 0.1613	R_1 = 0.041, wR_2 = 0.087
Largest diff. peak and hole /eÅ^{-3}	0.384 and -0.428	0.734 and -0.713	1.091 and -0.597	0.261 and -0.219	0.337 and -1.684
Absolute structure parameter	0.65(5)	-	-	-	-0.03(5)

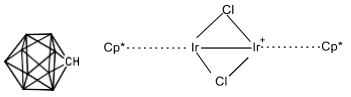
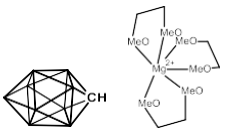
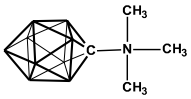
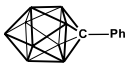
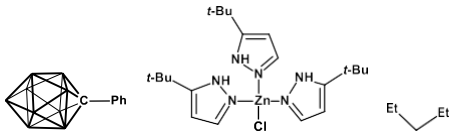
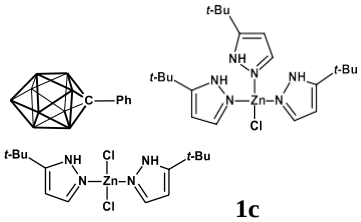
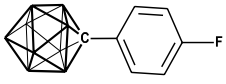
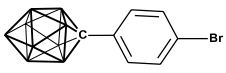
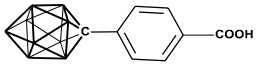
2. Crystal packing

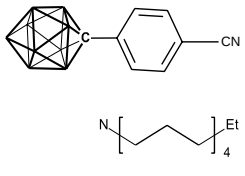
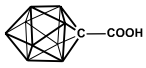
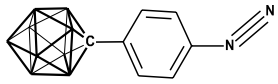
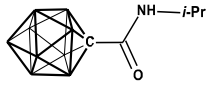
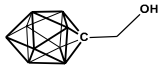
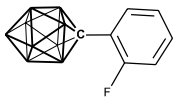
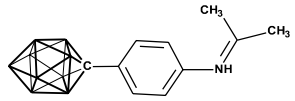
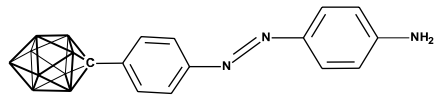
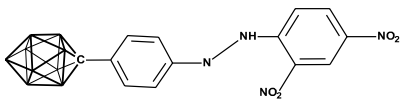
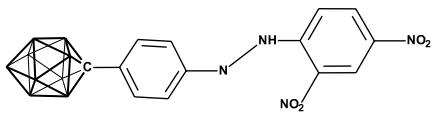
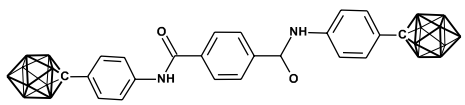
Table S2. Geometrical parameters for selected short intermolecular contacts. Atom numbers are given as in CIF files.

	Contact	Distance, Å	Distance-VdW, Å
Structure 1l[PyrCH$_2$Cl]	Cl1'···B10	3.711	-0.039
	C16'-H16'···B6	2.906	-0.294
	C16'-H16'···B6	2.993	-0.207
	C12-H12···B9'	2.725	-0.475
	C17-H17A···B8	3.074	-0.126
	C17-H17A···B10	3.024	-0.176
	C17'-H7A'···B6'	2.887	-0.313
	C17'-H7A'···B7'	2.670	-0.530
	C12-H12···B6'	2.766	-0.434
	C17'-H7A'···B10'	2.670	-0.516
	C12-H12···B2'	2.971	-0.229
	N19-H19A···Br20	2.511	-0.539
	N19'-H19D···Br20	2.541	-0.509
	N19-H19B···Br21	2.534	-0.516
Structure 1m[Et$_4$N]•[Et$_4$NBr]	C33-H33B···Br20	2.914	-0.136
	C41-H41B···Br20	2.900	-0.150
	C48-H48A···Br20	2.907	-0.143
	C19-H19A···Br20	2.511	-0.539
	C19'-H19D···Br20	2.541	-0.509
	C43-H43B···Br21	2.878	-0.172
	C61-H61A···B2	2.667	-0.533
	C83-H83B···B3	2.933	-0.267
	C83-H83B···B6	2.942	-0.258
Structure 1n	C12-H12B···B6	2.982	-0.218
	C12-H12B···B10	3.085	-0.115
	S11···B9	3.736	-0.064
	S11···B10	3.635	-0.165
	C13-H13B···B9	3.126	-0.074
Structure 1o	C13-H13···B9	2.931	-0.269
	C13-H13···B10	2.896	-0.304
	N16-H16···B6	2.781	-0.419
	N16-H16···B10	2.942	-0.258
	B6-H6···B5	3.134	-0.066
	C15(π)···B5	3.585	-0.115
	C15(π)···B7	3.534	-0.166
	C14(π)···B8	3.636	-0.064
	C15(π)···B8	3.541	-0.159
Structure 1q	B5-H5···I10	3.166	-0.014
	B2···B7	3.964	-0.036
	C2-H2···B7	3.164	-0.036

3. CSD search results

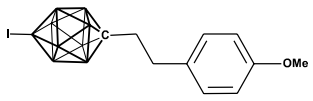
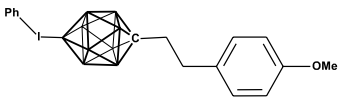
Table S3. Results of CSD (Cambridge Structural Database) search for derivatives of the [1-*closo*-$CB_9H_{10}]^-$ anion and its apical derivatives in series **1**. Filters used: 3D coordinates determined; No errors; Only organic substituents; Only single crystal structures.

Structure Diagram	CSD Refcode and Reference
 Y=H X=Any	
 **1a**	JOXCUU *K.Nestor, B.Stibr, J.D.Kennedy, M.Thornton-Pett, T.Jelinek* ***(1992)*** *Collect.Czech.Chem.Commun.,57,1262*
 **1a[MgL$_3$]**	LATRUW *S.G.McArthur, Rahul Jay, Linxiao Geng, Juchen Guo, V.Lavallo* ***(2017)*** *Chem.Commun. ,53,4453*
 **1b**	RUHZEZ *B.Stibr, J.Plesek, T.Jelinek, J.D.Kennedy, M.Thornton-Pett* ***(1997)*** *J.Chem.Soc.,Dalton Trans. ,4231*
 $[NEt_4]^+$ **1c[Et$_4$N]**	NEPKOI *T.Jelinek, C.A.Kilner, M.Thornton-Pett, J.D.Kennedy* ***(2001)*** *Chem.Commun ,1790*
 **1c**	WUKCOU *S.L.Renard, A.Franken, C.A.Kilner, J.D.Kennedy, M.A.Halcrow* ***(2002)*** *New J.Chem.,26,1634*
 **1c**	GOLTOS *S.L.Renard, A.Franken, J.D.Kennedy, C.A.Kilner, M.A.Halcrow* ***(2010)*** *CSD Communication (Private Communication)*
 $[N(CH_2)_6Et_4]^+$ **1d**	WECVAD *V.I.Bragin, A.A.Korlyukov, P.V.Petrovskii, I.B.Sivaev, V.I.Bregadze* ***(2012)*** *J.Fluorine Chem.,142,14*
 $[N(CH_2)_6Et_4]^+$ **1e**	JATMIB *I.B.Sivaev, Z.A.Starikova, P.V.Petrovskii, V.I.Bregadze, S.Sjoberg* ***(2005)*** *J.Organomet.Chem.,690,2790*
 $[NEt_4]^+$ **1f**	JAHNUC *A.Franken, M.J.Carr, W.Clegg, C.A.Kilner, J.D.Kennedy* ***(2004)*** *Dalton Trans.,3552*

 **1g**	DEKNUG *A.V.Shmalko, K.Yu.Suponitsky, I.B.Sivaev, V.I.Bregadze* ***(2022)*** *Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.) ,**71,** 399*
 $[NEt_4]^+$ **1h**	JAHPEO *A.Franken, M.J.Carr, W.Clegg, C.A.Kilner, J.D.Kennedy* ***(2004)*** *Dalton Trans.,3552*
 **1i**	AKABOD *A.Franken, C.A.Kilner, J.D.Kennedy* ***(2003)*** *Inorg.Chem.Commun.,**6,**1104*
 $[NEt_4]^+$ **1j**	GIJMUK *X. Liang, Y. Shen, K. Zhang, J. Liu, S. Duttwyler* ***(2018)*** *Chem.Commun.,54,12451*
 $[NEt_4]^+$ **1k**	JAHPOY *A.Franken, M.J.Carr, W.Clegg, C.A.Kilner, J.D.Kennedy* ***(2004)*** *Dalton Trans.,3552*
 $[N(CH_2)_6Et_4]^+$	WECTUV *V.I.Bragin, A.A.Korlyukov, P.V.Petrovskii, I.B.Sivaev, V.I.Bregadze* ***(2012)*** *J.Fluorine Chem.,142,14*
	AKABET *A.Franken, C.A.Kilner, J.D.Kennedy* ***(2003)*** *Inorg.Chem.Commun.,6,1104*
	AKABIX *A.Franken, C.A.Kilner, J.D.Kennedy* ***(2003)*** *Inorg.Chem.Commun.,6,1104*
 $[NEt_4]^+$ CH_3COOMe	JAHPUE *A.Franken, M.J.Carr, W.Clegg, C.A.Kilner, J.D.Kennedy* ***(2004)*** *Dalton Trans.,3552*
 $[NEt_4]^+$	JAHQAL *A.Franken, M.J.Carr, W.Clegg, C.A.Kilner, J.D.Kennedy* ***(2004)*** *Dalton Trans.,3552*
 $[NEt_4]^+$	ILITUS *N.J.Bullen, A.Franken, C.A.Kilner, J.D.Kennedy* ***(2003)*** *Chem.Commun. ,1684*

Y= F, Cl, Br, I X=Any

 $[NEt_4]^+$ **1p**	AWIMEY *A.Franken, C.A.Kilner, M.Thornton-Pett, J.D.Kennedy* ***(2002)*** *Collect.Czech.Chem.Commun.,**67,**869*

 $[NEt_4]^+$ **1v**	FUZROK *P.Kaszynski, R.Jakubowski, A.Pietrzak, A.C.Friedli* ***(2020)*** *Chem.-Eur.J.,26, 17481*
 **1u**	FUZRIE *P.Kaszynski, R.Jakubowski, A.Pietrzak, A.C.Friedli* ***(2020)*** *Chem.-Eur.J. ,26, 17481*
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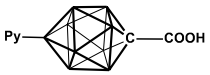
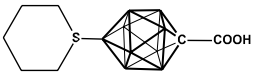
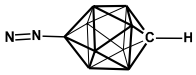
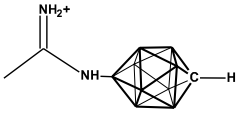
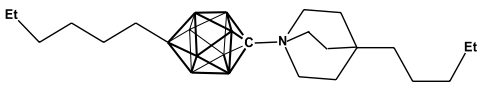
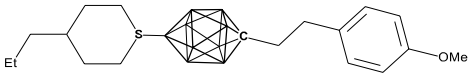
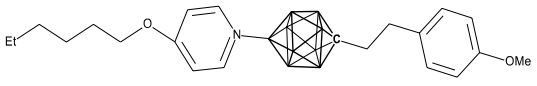
 **1s**	WAJKAV *B.Ringstrand, P.Kaszynski, V.G.Young Junior, Z.Janosuek* ***(2010)*** *Inorg.Chem.,49,1166*
 **1t**	WAJKID *B.Ringstrand, P.Kaszynski, V.G.Young Junior, Z.Janosuek* ***(2010)*** *Inorg.Chem. ,49,1166*
 **1w**	UFONOV *R.Zurawinski, R.Jakubowski, S.Domagala, P.Kaszynski, K.Wozniak* ***(2018)*** *Inorg.Chem.,57,10442*
 **1x**	UFOPAJ *R.Żurawinski, R.Jakubowski, S.Domagala, P.Kaszynski, K.Wozniak* ***(2018)*** *Inorg.Chem.,57,10442*
 **1y**	UFOPEN *R.Zurawinski, R.Jakubowski, S.Domagala, P.Kaszynski, K.Wozniak* ***(2018)*** *Inorg.Chem.,57,10442*
	SUJNOB *B.Ringstrand, P.Kaszynski, A.Januszko, V.G.Young Junior* ***(2009)*** *J.Mater.Chem.,19,9204*
	EMEQEV *R.Jakubowski, J.Pecyna, M.O.Ali, A.Pietrzak, A.C.Friedli, P.Kaszynski* ***(2021)*** *Dalton Trans.,50,3671*
	EMEQIZ *R.Jakubowski, J.Pecyna, M.O.Ali, A.Pietrzak, A.C.Friedli, P.Kaszynski* ***(2021)*** *Dalton Trans.,50,3671*

A total of 19 structures were selected for further analysis, mainly on the basis of simplicity of the substituents that could be effectively modeled with DFT methods and for which Hammett parameters are available. Also among three structures containing the 1-*closo*-CB_9H_9-1-Ph]$^-$ anion, structure **1c[Et$_4$N]** (NEPKOI)[5] was selected. Likewise, more recent structure **1a[MgL$_3$]** (LATRUW)[6] was selected for further studies.

4. Experimental and DFT structural parameters for series 1.

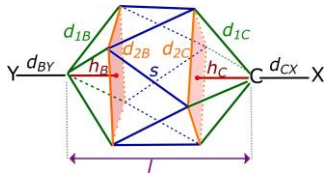


Figure S1. The structural model of the {*closo*-1-CB_9} skeleton in derivatives **1** with defined geometrical parameters.

Parameters d_{1B}, d_{2B}, s, d_{2C}, and d_{1C} are mean values of the equivalent bond lengths, 4 for all paramaters expect for s, which is an average of 8 values. For each average there is standard deviations given in parenthesis. Parameters h_B, h_C, d_{CX} and d_{CY} are unique values.

The torsion angles θ_X and θ_Y for the description of conformational properties are taken as absolute values and are defined for each class of derivatives shown in Figure S2 as shown below.

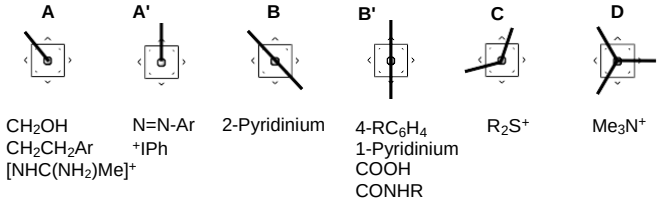


Figure S2. Conformational ground states for four types of substituents determined by DFT computational methods.

Class **A**: for substituent X at the C(1), θ_X defined by X_β–X_α–C(1)–B(2) atoms
for substituent Y at the B(10), θ_y defined by Y_β–Y_α–B(10)–B(9) atoms

Class **A'**: for substituent X at the C(1), θ_X defined by X_β–X_α–C(1)–B(6) atoms
for substituent Y at the B(10), θ_y defined by Y_β–Y_α–B(10)–B(2) atoms

Class **B**: for substituent X at the C(1), θ_X defined by an average of two related values

$\theta_X = ½(|\theta_X'|+ |\theta_X''|)$

θ_X' defined by X_β'–X_α'–C(1)–B(2) atoms

θ_X" defined by X_β"–X_α"–C(1)–B(4) atoms

for substituent Y at the B(10), θ_Y defined by an average of two related values

$\theta_Y = ½(|\theta_Y'|+ |\theta_Y''|)$

θ_Y' defined by Y_β'–Y_α'–B(10)–B(9) atoms

θ_Y'' defined by Y_β''–Y_α''–B(10)–B(7) atoms

Class **B'**: for substituent X at the C(1), θ_X defined by an average of two related values

$\theta_X = ½(|\theta_X'|+ |\theta_X''|)$

θ_X' defined by X_β'–X_α'–C(1)–B(6) atoms

θ_X'' defined by X_β''–X_α''–C(1)–B(8) atoms

for substituent Y at the B(10), θ_Y defined by an average of two related values

$\theta_Y = ½(|\theta_Y'|+ |\theta_Y''|)$

θ_Y' defined by Y_β'–Y_α'–B(10)–B(5) atoms

θ_Y'' defined by Y_β''–Y_α''–B(10)–B(3) atoms

Class **C**: for substituent X at the C(1), θ_X defined by a differnce of two related values

$\theta_X = |\theta_X'|– |\theta_X''|$

θ_X' defined by X_β'–X_α'–C(1)–B(2) atoms

θ_X'' defined by X_β''–X_α''–C(1)–B(2) atoms

for substituent Y at the B(10), θ_Y defined by an average of two related values

$\theta_Y = |\theta_Y'|– |\theta_Y''|$

θ_Y' defined by Y_β'–Y_α'–B(10)–B(9) atoms

θ_Y'' defined by Y_β''–Y_α''–B(10)–B(9) atoms

Class **D**: for substituent X at the C(1), θ_X defined by X_β–X_α–C(1)–B(2) atoms

for substituent Y at the B(10), θ_y defined by Y_β–Y_α–B(10)–B(9) atoms

The results are shown in Table S4 for experimental data and in Table S5 for DFT-optimized geometries.

Table S4. Experimental structural parameters (Figures S1 and S2) describing the geometry of the {*closo*-1-CB_9} cluster.

Experimental parameters												
	d_{1B}	d_{2B}	h_B	s	h_C	d_{2C}	d_{1C}	l	d_{CX}	d_{BY}	Θ_X	Θ_Y
1a LATRUW	1.697(3)	1.839(6)	1.090	1.805(4)	0.933	1.834(2)	1.597(4)	3.529	0.97	1.1200	…	…
1b RUHZEZ	1.697(1)	1.839(8)	1.090	1.801(1)	0.937	1.846(6)	1.607(4)	3.526	1.501	1.1160	0.0	…
1c NEPKOI	1.698(3)	1.837(4)	1.094	1.808(4)	0.943	1.838(4)	1.606(5)	3.546	1.503	1.1210	9.1 [a]	…
1d WECVAD	1.69(7)	1.81 (1)	1.101	1.77(2)	0.947	1.89(5)	1.62(2)	3.508	1.477	1.061	7.6 [a]	…
1e JATMIB	1.693(7)	1.832(4)	1.091	1.808(9)	0.948	1.834(6)	1.606(4)	3.550	1.494	1.1320	13.5 [a]	…
1f JAHNUC	1.698(5)	1.838(2)	1.093	1.801(8)	0.948	1.84(1)	1.608(5)	3.543	1.492	1.1200	1.3 [a]	…
1g DEKNUG	1.702(3)	1.840(5)	1.097	1.807(3)	0.959	1.845(6)	1.619(5)	3.564	1.481	1.09	1.7 [a]	…
1h JAHPEO	1.71(2)	1.845(8)	1.101	1.811(9)	0.934	1.86(1)	1.613(5)	3.543	1.484	1.1200	0.0 [a]	…
1i AKABOD	1.704(2)	1.844(2)	1.097	1.807(3)	0.945	1.847(6)	1.612(4)	3.547	1.477	1.1200	6.2 [a]	…
1j GIJMUK	1.69(1)	1.83(1)	1.085	1.797(9)	0.944	1.836(7)	1.605(3)	3.527	1.486	1.1260	37.3 [a]	…
1k JAHPOY	1.697(2)	1.8339(4)	1.095	1.804(6)	0.944	1.836(4)	1.605(1)	3.545	1.522	1.1195	47 [b]	…
1l[PyrCH$_2$Cl]	1.701(2)	1.843(2)	1.093	1.805(4)	0.924	1.850(3)	1.602(4)	3.520	1.741	1.0650	…	…
1m[Et$_4$N]•[Et$_4$NBr]	1.691(4)	1.832(3)	1.087	1.806(4)	0.932	1.84 (1)	1.603(3)	3.526	1.441	1.1195	4.8 [a]	…
1n	1.695(5)	1.848(4)	1.080	1.800(4)	0.941	1.858(8)	1.616(5)	3.515	1.765	1.1200	8.3 [c]	…
1o	1.699(4)	1.841(2)	1.091	1.801(5)	0.943	1.85(1)	1.611(2)	3.533	1.466	1.1480	27.0 [a]	…
1p AWIMEY	1.692(5)	1.849(3)	1.074	1.8043(8)	0.950	1.845(4)	1.614(2)	3.526	1.486	2.1630	1.1 [a]	…
1q	1.69(1)	1.864(7)	1.056	1.804(6)	0.929	1.896(5)	1.622(3)	3.458	1.385	2.1490	…	…
1r WAJKEZ	1.670(2)	1.879(6)	1.013	1.805(2)	0.922	1.859(7)	1.606(1)	3.429	1.4860	1.498	5.7 [a]	…
1s WAJKAV	1.677(2)	1.849(4)	1.048	1.799(4)	0.927	1.847(6)	1.602(2)	3.471	1.4818	1.52525	13.7 [d]	7.9 [d]
1t WAJKID	1.680(3)	1.858(1)	1.048	1.805(4)	0.930	1.85(1)	1.607(3)	3.478	1.4850	1.858	15.7 [c]	47.6 [c, a]
1u FUZRIE	1.675(2)	1.864(8)	1.033	1.809(4)	0.942	1.842(5)	1.608(2)	3.482	1.517	2.178	22.5	14.6
1v FUZROK	1.696(4)	1.854(7)	1.076	1.815(3)	0.946	1.843(2)	1.611(2)	3.536	1.519	2.1650	21.2	…
1w UFONOV	1.6748(2)	1.8755(9)	1.022	1.810(1)	0.923	1.853(3)	1.6023(9)	3.448	1.094	1.4940	…	…
1x UFOPAJ	1.686(4)	1.855(4)	1.059	1.809(2)	0.929	1.849(4)	1.604(2)	3.494	0.965	1.5260	…	28.4 [a]
1y UFOPEN	1.698(3)	1.846(2)	1.086	1.806(4)	0.932	1.845(5)	1.603(1)	3.523	0.947	1.5030	…	30.9

[a] Average of two values.
b Two independent molecule. Average of four values
[c] Difference of two values.
d Average of 8 values for 4 independent molecules.

Table S5. DFT-derived structural parameters (Figures S1 and S2) describing the geometry of the {*closo*-1-CB_9} cluster.

DFT parameters												
	d_{1B}	d_{2B}	h_B	s	h_C	d_{2C}	d_{1C}	l	d_{CX}	d_{BY}	Θ_X	Θ_Y
1a LATRUW	1.6964(0)	1.8380(0)	1.090	1.8032(0)	0.932	1.8393(0)	1.5998(0)	3.5257	1.0767	1.1885	--	--
1b RUHZEZ	1.6963(0)	1.843(1)	1.086	1.795(3)	0.938	1.848(4)	1.608(3)	3.5155	1.5078	1.1845	0.0	--
1c NEPKOI	1.6967(5)	1.838(0)	1.090	1.8003(8)	0.954	1.835(3)	1.6108(0)	3.5455	1.4855	1.1879	0.0	--
1d WECVAD	1.6967(6)	1.838(0)	1.090	1.8002(9)	0.953	1.836(3)	1.6106(0)	3.5447	1.4851	1.1877	0.0	--
1e JATMIB	1.6968(4)	1.8386(0)	1.090	1.8000(8)	0.953	1.8364(4)	1.6107(0)	3.5436	1.4835	1.1876	0.0	--
1f JAHNUC	1.697(2)	1.8404(6)	1.089	1.7987(7)	0.941	1.85(1)	1.6088(0)	3.5269	1.4789	1.1872	0.0	--
1g DEKNUG	1.6970(2)	1.8392(0)	1.090	1.7994(8)	0.952	1.838(5)	1.6110(0)	3.5413	1.4799	1.1873	0.0	--
1h JAHPEO	1.697(2)	1.8404(6)	1.089	1.7987(7)	0.941	1.85(1)	1.6088(0)	3.5269	1.4789	1.1872	0.0	--
1i AKABOD	1.699(2)	1.8420(0)	1.091	1.796(1)	0.950	1.845(1)	1.6140(0)	3.5343	1.4615	1.1854	0.0	--
1j GIJMUK	1.697(1)	1.839(1)	1.090	1.800(3)	0.945	1.840(6)	1.608(2)	3.5346	1.5002	1.1876	12.1 [a]	--
1k JAHPOY	1.696(1)	1.8383(9)	1.090	1.802(2)	0.946	1.835(6)	1.606(3)	3.5386	1.505	1.1885	0.0	--
1l	1.6957(0)	1.8414(0)	1.086	1.8007(0)	0.923	1.8487(0)	1.600(0)	3.5076	1.7572	1.1869	--	--
1m	1.697(2)	1.8404(6)	1.089	1.800(1)	0.940	1.84(1)	1.607(1)	3.5274	1.4273	1.1877	0.0	--
1n	1.6977	1.844(3)	1.087	1.796(2)	0.930	1.856(5)	1.609(4)	3.5075	1.7688	1.1843	0.0 [b]	--
1o	1.699(2)	1.843(3)	1.090	1.795(2)	0.947	1.8468(7)	1.613(5)	3.5290	1.4623	1.1846	0.0	--
1p AWIMEY	1.6863(6)	1.8476(0)	1.066	1.8006(8)	0.950	1.838(3)	1.6099(0)	3.5158	1.4862	2.1932	0.0	--
1q	1.6992(0)	1.8579(0)	1.078	1.7880(0)	0.921	1.8876(0)	1.6217(0)	3.4716	1.3519	2.1562	--	--
1r WAJKEZ	1.675(1)	1.8761(3)	1.022	1.8002(5)	0.924	1.857(8)	1.6053(2)	3.4362	1.4913	1.471	0.0	--
1s WAJKAV	1.681(1)	1.853(2)	1.052	1.799(1)	0.931	1.851(9)	1.6060(6)	3.4765	1.485	1.5264	1.2 [a]	0.0
1t WAJKID	1.6794(3)	1.856(2)	1.048	1.800(5)	0.930	1.85(1)	1.606(3)	3.4718	1.4866	1.8721	0.0	0.0 [b]
1u FUZRIE	1.670(2)	1.862(6)	1.026	1.803(3)	0.943	1.839(3)	1.606(3)	3.4690	1.5178	2.2121	10.3	12.1
1v FUZROK	1.6856(8)	1.847(2)	1.066	1.802(2)	0.949	1.834(1)	1.607(1)	3.5166	1.5166	2.1955	10.7	--
1w UFONOV	1.6753(0)	1.8740(0)	1.025	1.803(0)	0.915	1.8520(0)	1.5978(0)	3.4351	1.0763	1.4686	--	--
1x UFOPAJ	1.6804(0)	1.851(2)	1.054	1.802(6)	0.923	1.8455(0)	1.592(6)	3.4750	1.0761	1.5277	--	0.0
1y UFOPEN	1.690(6)	1.8460(9)	1.073	1.801(5)	0.924	1.844(7)	1.5984(6)	3.4964	1.0761	1.5058	--	9.4

[a] Average of two values.
[b] Difference of two values.

5. Additional correlations of experimental and DFT structural parameters

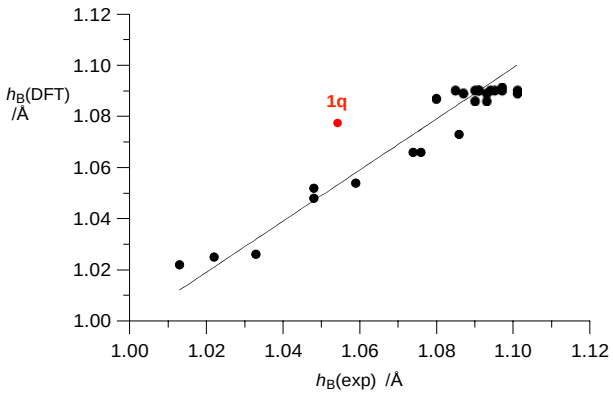


Figure S3. Correlation of experimental and DFT–derived geometrical parameter h_B for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoint for **1q** (red): $h_{B(DFT)} = h_{B(exp)} - 0.001(1)$, $r^2 = 0.925$. With **1q** $r^2 = 0.883$.

The experimental value $h_{B(exp)}$ for **1q** exhibits the largest difference from the predicted based on the general correlation of 0.023 Å, while the average absolute difference for this set of parameter is 0.005 Å. The second largest deviation from the prediction is for **1y** (0.012 Å).

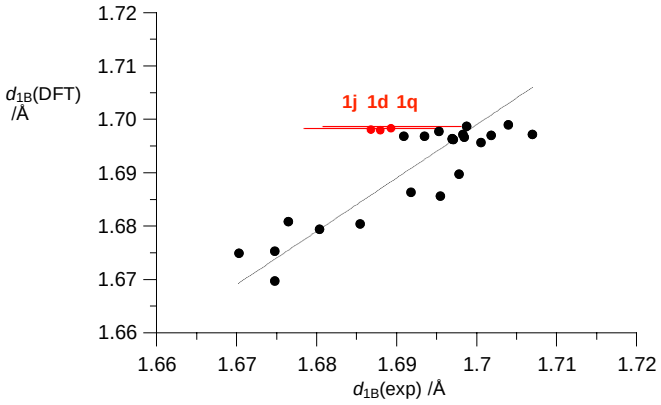


Figure S4. Correlation of experimental and DFT–derived geometrical parameter d_{1B} for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoints for **1d**, **1j**, and **1q**: $d_{1B(DFT)} = d_{1B(exp)} - 0.001(1)$, $r^2 = 0.76$. The horizontal red lines represent error bars with 1σ.

The average absolute difference for this set of parameter is 0.0035 Å. Value $d_{1B(exp)}$ for the three derivatives **1d**, **1j**, and **1q** differ from the predicted by about 0.01 Å, which is comparable with the *std* for the last two average parameters. The *std* value for **1d** is 0.07 Å, which is covers a wide range of $d_{1B(exp)}$ values, from 1.61–1.75 Å.

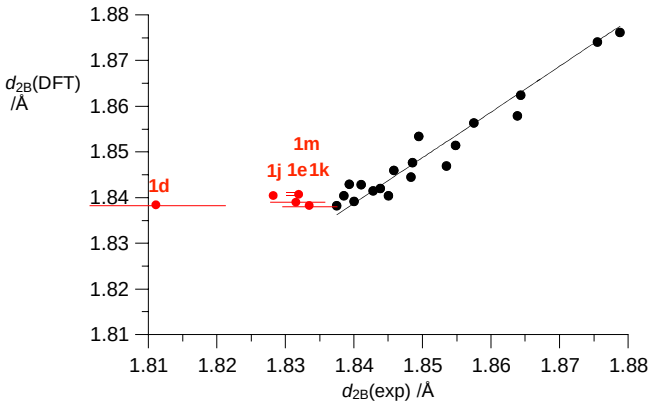


Figure S5. Correlation of experimental and DFT–derived geometrical parameter d_{2B} for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoints for **1d**, **1e**, **1j**, **1k** and **1m** (red): $d_{2B(DFT)} = d_{2B(exp)} - 0.001(1)$, $r^2 = 0.76$. The horizontal red lines represent error bars with 1σ.

The experimental value $d_{2B(exp)}$ for **1d** exhibits the largest difference from the predicted based on the general correlation of 0.027 Å, while the average absolute difference for this set of parameter is 0.0025 Å. Also the $d_{2B(exp)}$ value for **1j** significantly deviate from the predicted by 0.013 Å, which is close to the *std* value for this parameter (0.01 Å). Three derivatives **1e**, **1m**, and **1k** deviate much less from the expected values (0.005–0.009 Å) and could be included in the correlation. Their *std* is 0.002 and 0.004 Å.

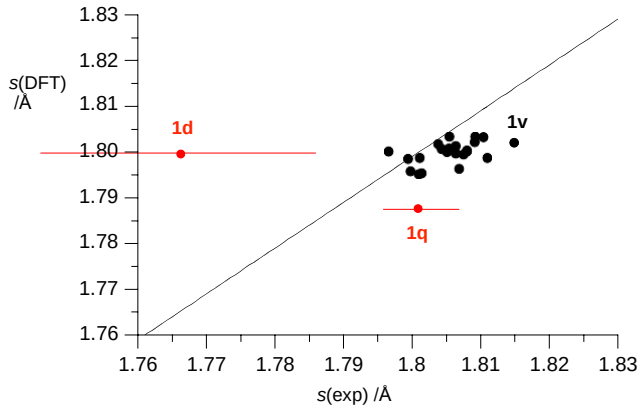


Figure S6. Correlation of experimental and DFT–derived geometrical parameter *s* for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoints for **1d** and **1q**: $s_{(DFT)} = s_{(exp)} - 0.001(1)$, $r^2 = 0.999$. The horizontal red lines represent error bars with 1σ.

The experimental value $s_{(exp)}$ for **1d** exhibits the largest difference of 0.032 Å from the predicted based on the general correlation, while the average absolute difference for this set of parameter is 0.005 Å. Derivative **1q** deviate from the expected value by 0.0145 Å with the *std* of 0.006 Å. The remaining datapoints cluster close to the fitting line.

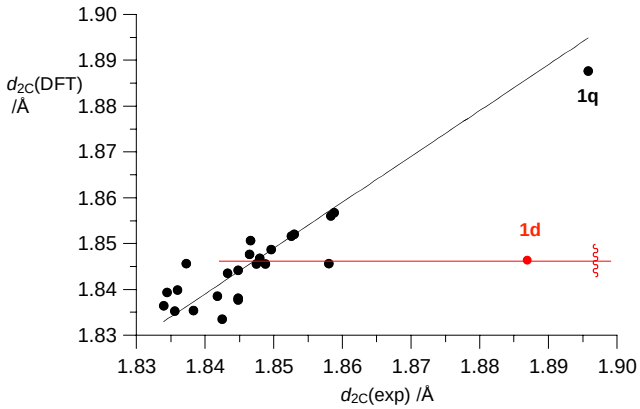


Figure S7. Correlation of experimental and DFT–derived geometrical parameter d_{2C} for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoint for **1d** (red): $d_{2C(DFT)} = d_{2C(exp)} - 0.001(1)$, $r^2 = 0.81$. The horizontal red line represents the error bar with 1σ.

Only the experimental value d_{2C} for **1d** does not conform to the general fitting line with the difference of 0.045 Å, while the average absolute difference for this set of parameter is 0.003 Å.

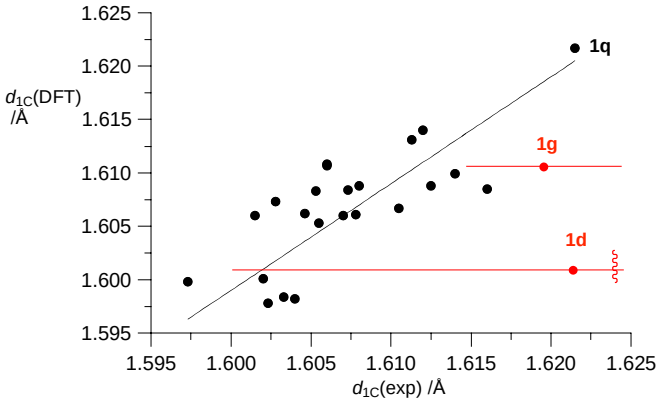


Figure S8. Correlation of experimental and DFT–derived geometrical parameter d_{1C} for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line excluding datapoints for **1d**, **1g**, and **1r** (red): $d_{1C(DFT)} = d_{1C(exp)} - 0.001(1)$, $r^2 = 0.56$. The horizontal red line represents the error bar with 1σ.

The experimental value d_{1C} for **1d** exhibits a large difference (0.011 Å) from the value predicted based on the general correlation, while the average absolute difference for this set of parameter is 0.003 Å. Also the d_{1C} value for **1g** deviate from the predicted by 0.009 Å.

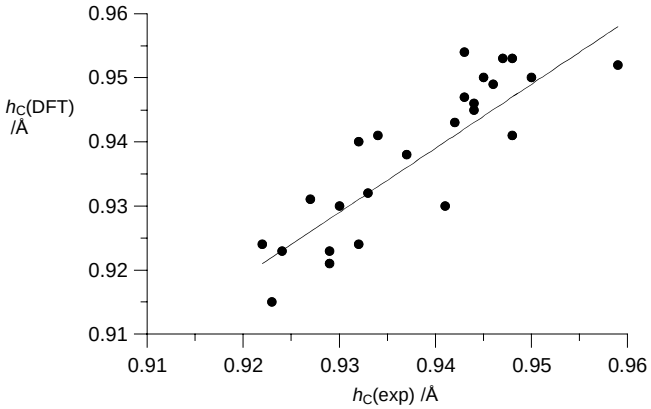


Figure S9. Correlation of experimental and DFT–derived geometrical parameter h_C for the {*closo*-1-CB_9} cluster in series **1** as defined in Figure S1. Best fitting line: $h_{C(DFT)} = h_{C(exp)} - 0.001(1)$, $r^2 = 0.75$.

No particular outliers in this correlation. The mean absolute difference between the experimental and DFT h_C values is 0.005 Å.

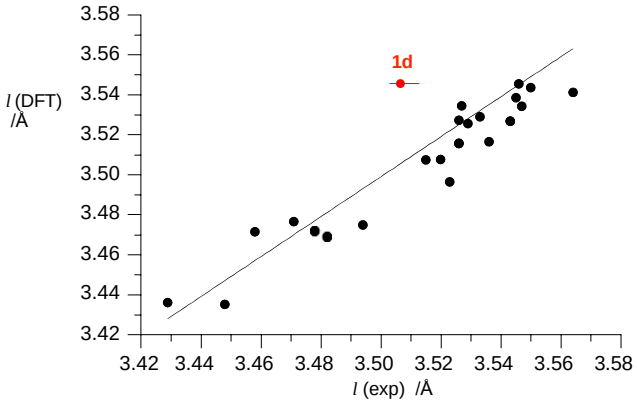


Figure S10. Correlation of experimental and DFT–derived geometrical parameter *l* for the {*closo*-1-CB_9} cluster in series **1** (no **1d**) as defined in Figure S1. Fitting to the general correlation line $l_{(DFT)} = l_{(exp)} - 0.001(1)$ without **1d**: $r^2 = 0.86$.

6. Hammett constants used in structural analysis

For the purpose of this work, Hammett parameters for 4-X-C_6H_4 substituents were derived from correlation shown in Figure S11. All σ_p parameters used in this work are listed in Table S6.

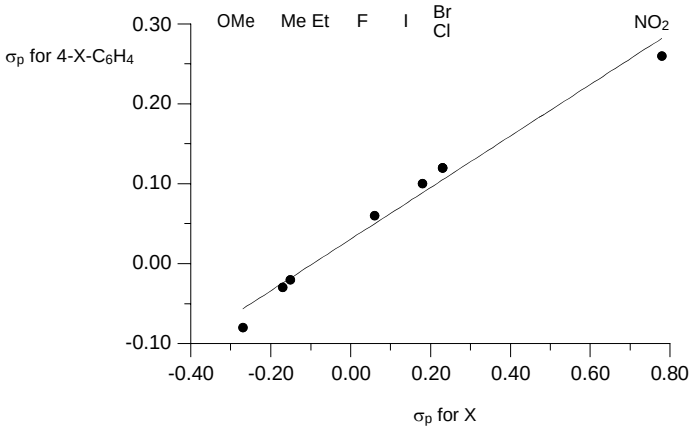


Figure S11. Correlation of Hammett parameter σ_p for substituents X and 4-XC_6H_4-. Best fitting line: $\sigma_{p(XC6H4)}$ = 0.323(20) $\cdot\sigma_{p(X)}$ + 0.030(6), r^2 = 0.979.

Table S6. Hammett substituent constants used in the analysis; σ_X constant for substituent at the C(1) position, σ_Y constant for substituent at the B(10) position, σ_{X+Y} sum of the two Hammett constants.

compound	C–X	B–Y	σ_X	σ_Y	$\sigma_X+\sigma_Y$	ref [a]
1a	H	H	0.00	0.00	0.00	definition
1b	NMe_3^+	H	0.82	0.00	0.82	[7]
1c	Ph	H	-0.01	0.00	-0.01	[7]
1d	C_6H_4F-4	H	0.06	0.00	0.06	[7]
1e	C_6H_4Br-4	H	0.12	0.00	0.12	[7]
1f	C_6H_4COOH-4	H	0.18	0.00	0.18	this work
1g	C_6H_4CN-4	H	0.24	0.00	0.24	this work
1h	COOH	H	0.45	0.00	0.45	[7]
1i	$C_6H_4N_2^+$-4	H	0.64	0.00	0.64	this work
1j	CONHPr-*i*	H	0.36 [b]	0.00	0.36	
1k	CH_2OH	H	0.00	0.00	0.00	[7]
1l	Cl	H	0.23	0.00	0.23	[7]
1m	N=N-$C_6H_4NH_2$-4	H	0.31 [c]	0.00	0.31	
1n	SMe_2^+	H	0.90	0.00	0.90	[7]
1o	2-$C_5H_5N^+$	H	–	0.00	–	
1p	Ph	I	-0.01	0.18	0.17	[7]
1q	N_2^+	I	1.91	0.18	2.09	[7]
1r	COOH	N_2^+	0.45	1.91	2.36	[7]
1s	COOH	1-$C_5H_5N^+$	0.45	0.82	1.27	[7-8]
1t	COOH	1-$S(CH_2)_5^+$	0.45	0.90 [d]	1.35	[7]
1u	$CH_2CH_2C_6H_4OMe$-4	PhI^+	-0.12 [e]	1.50	1.38	[8]
1v	$CH_2CH_2C_6H_4OMe$-4	I	-0.12 [e]	0.18	0.06	
1w	H	N_2^+	0.00	1.91	1.91	[7]
1x	H	1-$C_5H_5N^+$	0.00	0.82	0.82	[8]
1y	H	$NHC(=NH_2)Me^+$	0.00	0.48	0.48	[8]

[a] Values for individual groups are taken form ref [7] unless indicated otherwise. [b] Value for COONHMe ref[7]. [c] Value for N=N-C_6H_3-2-OH-5-Me, ref [7]. [d] Value for SMe_2^+, ref [7]. [e] Value for CH_2CH_2Ph, ref [7]

7. Additional correlations of geometrical parameters with Hammett constants

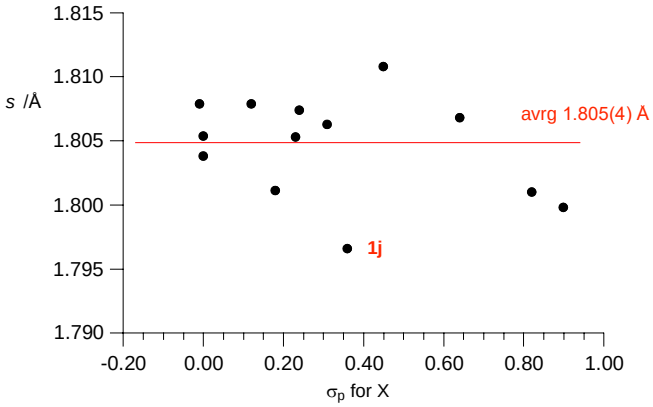


Figure S12. A plot of parameter *s vs* σ_p values for substituents at the C(1) in series **1a**–**1n** (no **1d**).

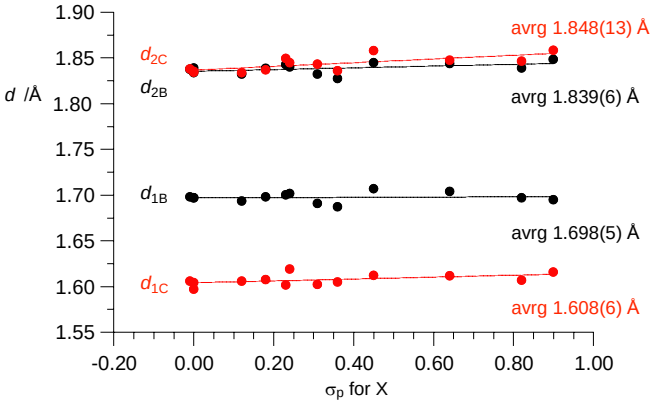


Figure S13. A plot of parameters d_C and d_B *vs* σ_p values for substituents at the C(1) in series **1a**–**1n** (no **1d**).

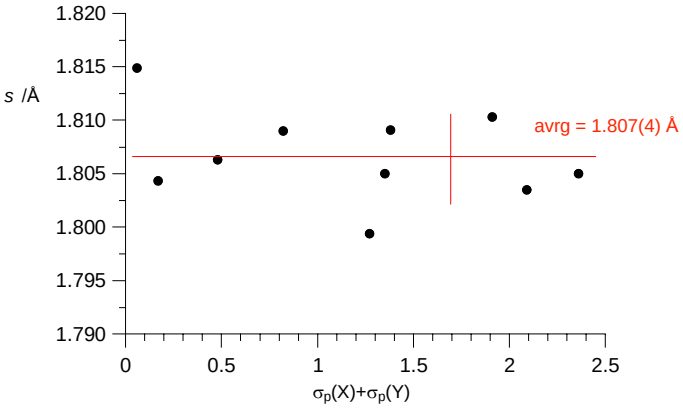


Figure S14. A plot of parameters *s vs* sum of σ_p(X) and σ_p(Y) values in series **1p**–**1y**. The horizontal red line represents the average value, while the vertical shows *std* for the average.

8. Archive for DFT results

1a


```
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H10B9(1-)\PIOTR\26-Sep-2021\
 0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S
 CRF(Solvent=C6H5Cl)\\1-CB10 parent anion, C4v\\-1,1\B,-1.3005599386,0.
 ,-0.5273135462\B,0.,1.3005599386,-0.5273135462\B,1.3005599386,0.,-0.52
 73135462\B,0.,-1.3005599386,-0.5273135462\B,-0.9190159841,-0.919015984
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 1,0.9190159841,0.9765035343\B,0.9190159841,-0.9190159841,0.9765035343\
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 407,-1.7134978407,1.376958959\\Version=ES64L-G09RevD.01\State=1-A1\HF=
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 rupole=-0.50885,-0.50885,1.0177,0.,0.,0.\PG=C04V     [C4(H1B1C1H1),2SGV(H2
 B2),2SGD(H2B2)]\\@
```


1b


```
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 \#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
 F(Solvent=C6H5Cl) freq(noraman, readIso)\\1-CB9 1-NMe3, Cs\\0,1\B,1.43
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 4,2.6909900921,0.\C,-0.1713350871,-0.3405685896,0.\N,-0.9808310326,-1.
 6126823227,0.\C,-0.0914857158,-2.825940503,0.\B,0.3135940799,0.4636672
 108,1.3064026777\B,0.3135940799,0.4636672108,-1.3064026777\B,1.8552442
 679,1.287527442,-0.9219232092\B,1.8552442679,1.287527442,0.9219232092\
 B,0.2653819195,2.2203618537,0.920646695\B,0.2653819195,2.2203618537,-0
 .920646695\C,-1.8689010778,-1.6820965371,1.2166857839\C,-1.8689010778,
 -1.6820965371,-1.2166857839\H,2.2123961074,3.7101735576,0.\H,2.1117873
 581,-1.1643493268,0.\H,-2.0002310503,1.2271282085,0.\H,-0.7277295679,-
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 5\H,-1.2492737423,-1.7166251649,-2.1046039715\H,-1.2492737423,-1.71662
 51649,2.1046039715\H,-2.5042666923,-0.8027540721,1.2353220715\H,-2.504
 2666923,-0.8027540721,-1.2353220715\H,0.5293446306,-2.8078565493,-0.88
 93145144\H,0.5293446306,-2.8078565493,0.8893145144\\Version=ES64L-G09R
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```


1c


```
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 7,-0.9160778973,-1.1350814636\B,-0.9193049737,0.9160778973,-1.13508146
 36\B,0.9193049737,0.9160778973,-1.1350814636\B,0.9193049737,-0.9160778
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]\\@

1d

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3\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
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H4B4)]\\@

1e

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H9B9Br1(1-)\PIOTR\29-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl)\\1-CB9-1-Br, C4v\\-1,1\B,-1.3073768887,0.,-0.014
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8\B,0.,-1.3073768887,-0.0142463228\B,-0.9207175138,-0.9207175138,1.484
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,-1.7143103716,1.8842389053\\Version=ES64L-G09RevD.01\State=1-A1\HF=-2
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V(H2B2),2SGD(H2B2)]\\@

1f

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277574015,-0.9299670253,-0.9158146285\B,4.8204080665,-0.0172441984,0.\
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934549901,1.2329215381,0.\C,-2.3204437365,-1.1750533229,0.\C,-0.909854
0225,1.21605134,0.\C,-0.9348877638,-1.1853575979,0.\C,-3.0167629196,0.
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C,-4.4936730786,0.1013143524,0.\O,-5.1478959639,1.1227629862,0.\O,-5.0
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5.2093119,8.7021167,0.,0.\PG=CS [SG(C8H8B3O2),X(H6B6)]\\

1g

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C8H13B9N1(1-)\PIOTR\11-Jan-202
3\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl) freq(noraman, readIso)\\1-CB9 1-Ph-4-CN, C2v\\-1
,1\B,0.,1.3012244687,-3.3403973204\B,0.,-1.3012244687,-3.3403973204\B,
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1349,0.9216769732,-1.8400048259\B,0.9163411349,0.9216769732,-1.8400048
259\B,0.9163411349,-0.9216769732,-1.8400048259\B,-0.9163411349,-0.9216
769732,-1.8400048259\B,0.,0.,-4.429466771\C,0.,0.,-0.8881511086\C,0.,0
.,0.5917901407\C,0.,1.2096490421,2.6941343701\C,0.,-1.2096490421,2.694
1343701\C,0.,1.2014183372,1.3101738754\C,0.,-1.2014183372,1.3101738754
\C,0.,0.,3.3989896112\H,0.,2.4232602869,-3.7420336158\H,0.,-2.42326028
69,-3.7420336158\H,2.4239389506,0.,-3.7332218959\H,-2.4239389506,0.,-3
.7332218959\H,-1.6782349698,1.6763385313,-1.3320428253\H,1.6782349698,
1.6763385313,-1.3320428253\H,1.6782349698,-1.6763385313,-1.3320428253\
H,-1.6782349698,-1.6763385313,-1.3320428253\H,0.,0.,-5.6167372246\H,0.
,2.1470796301,3.2339093503\H,0.,-2.1470796301,3.2339093503\H,0.,2.1402
971849,0.7732744803\H,0.,-2.1402971849,0.7732744803\C,0.,0.,4.82604370
28\N,0.,0.,5.9802191611\\Version=ES64L-G09RevD.01\State=1-A1\HF=-591.5
643711\RMSD=7.488e-09\RMSF=2.001e-06\Dipole=0.,0.,3.1833517\Quadrupole
=20.7022706,27.5544588,-48.2567294,0.,0.,0.\PG=C02V [C2(H1B1C1C1C1C1N1
),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\@

1h

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C2H10B9O2(1-)\PIOTR\27-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl) freq(noraman, readIso)\\CB9H9-1-COOH, Cs\\-1,1\B
,1.7042900366,-0.234233542,0.\B,-0.5052746981,-1.6136418695,0.\B,0.596
2011416,-0.9170756676,1.3002958825\B,0.5962011416,-0.9170756676,-1.300
2958825\B,0.5931750503,0.8413832849,-0.9167998781\B,0.5931750503,0.841
3832849,0.9167998781\B,-0.9814728089,-0.1422571519,0.9178116238\B,-0.9
814728089,-0.1422571519,-0.9178116238\B,1.1745454368,-1.8448570693,0.\
H,1.8035009186,-2.8517503784,0.\C,-0.6928083574,1.1471506336,0.\C,-1.4
425433681,2.4219287289,0.\H,-3.1880633334,3.1244934781,0.\O,-0.9493996
994,3.5266882495,0.\O,-2.7814420423,2.2429481503,0.\H,2.8694736814,0.0
136101374,0.\H,-1.2407619447,-2.5509760715,0.\H,0.8061072623,-1.255084
2939,2.4232918802\H,0.8061072623,-1.2550842939,-2.4232918802\H,0.96020
10019,1.673311637,-1.6763668641\H,0.9602010019,1.673311637,1.676366864
1\H,-1.8876939603,-0.1110501426,1.6805860649\H,-1.8876939603,-0.111050
1426,-1.6805860649\\Version=ES64L-G09RevD.01\State=1-A'\HF=-456.801906
\RMSD=6.112e-09\RMSF=1.744e-05\Dipole=-1.9213405,1.7015185,0.\Quadrupo
le=3.9020381,-7.7426798,3.8406417,-0.2777433,0.,0.\PG=CS [SG(C2H4B3O2)
,X(H6B6)]\\

1i

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H13B9N2\PIOTR\27-May-2022\0\
\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
F(Solvent=C6H5Cl) freq(noraman, readIso)\\1-CB9 1-Ph-4-N2, C2v\\0,1\B,
0.,1.303141187,-3.3204242293\B,0.,-1.303141187,-3.3204242293\B,1.30183
35863,0.,-3.3117247453\B,-1.3018335863,0.,-3.3117247453\B,-0.915530173
3,0.9299036076,-1.822384455\B,0.9155301733,0.9299036076,-1.822384455\B
,0.9155301733,-0.9299036076,-1.822384455\B,-0.9155301733,-0.9299036076
,-1.822384455\B,0.,0.,-4.4070013139\C,0.,0.,-0.872688019\C,0.,0.,0.588
7761624\C,0.,1.2354304533,2.6769896239\C,0.,-1.2354304533,2.6769896239

\C,0.,1.2144515726,1.3042869255\C,0.,-1.2144515726,1.3042869255\C,0.,0
.,3.3485254415\H,0.,2.4223575171,-3.7247560253\H,0.,-2.4223575171,-3.7
247560253\H,2.4240004905,0.,-3.7072071774\H,-2.4240004905,0.,-3.707207
1774\H,-1.6753627843,1.6805954942,-1.3075956756\H,1.6753627843,1.68059
54942,-1.3075956756\H,1.6753627843,-1.6805954942,-1.3075956756\H,-1.67
53627843,-1.6805954942,-1.3075956756\H,0.,0.,-5.5923094987\H,0.,2.1619
709752,3.2327781968\H,0.,-2.1619709752,3.2327781968\H,0.,2.1479007597,
0.7604061947\H,0.,-2.1479007597,0.7604061947\N,0.,0.,4.7097816315\N,0.
,0.,5.8141928821\\Version=ES64L-G09RevD.01\State=1-A1\HF=-608.0009631\
RMSD=5.349e-09\RMSF=1.626e-06\Dipole=0.,0.,9.9479919\Quadrupole=-6.720
5934,2.5710609,4.1495325,0.,0.,0.\PG=C02V [C2(H1B1C1C1C1N1N1),SGV(C4H6
B2),SGV'(H2B2),X(H4B4)]\\@

1j

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C5H17B9N1O1(1-)\PIOTR\30-May-2
022\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck
#P SCRF(Solvent=C6H5Cl)\\CB9H9-1-CONH-i-Pr, C1\\-1,1\B,-2.3208578717,1
.0873196761,0.2717462237\B,-1.9391984528,-1.4291959263,-0.2722905014\B
,-2.1649651589,0.1005371608,-1.2709192916\B,-2.0890941414,-0.440303981
1,1.2711490283\B,-0.7532397743,0.7601645959,1.0946297368\B,-0.80802752
44,1.1393402288,-0.7009482834\B,-0.5372686608,-0.6443488005,-1.0870499
652\B,-0.4872430565,-1.0244523635,0.7049290436\B,-3.2057625845,-0.3338
07052,-0.0021392306\H,-4.3799929256,-0.51162435,-0.005235823\C,0.28807
73991,0.2012958713,0.0067711155\C,1.7653320953,0.4627281626,0.01196735
84\O,2.2287120742,1.6000786005,0.0130484317\H,-2.885522113,2.110269826
7,0.5057113252\H,-2.171085649,-2.5746655255,-0.5071265036\H,-2.5910781
723,0.2743113694,-2.3702546055\H,-2.4475734834,-0.7343966857,2.3690728
634\H,-0.3418322709,1.4054347798,2.0001528909\H,-0.4462665332,2.101876
8907,-1.2886088404\H,0.055245213,-1.1440449107,-1.9860266179\H,0.14342
11175,-1.8413888647,1.2928356992\N,2.5392084456,-0.6486210328,0.012699
1412\C,3.9988679523,-0.6410388938,0.0208352683\H,2.0707458222,-1.54087
92201,0.0356096316\H,4.2800369672,0.4114872559,0.0312047299\C,4.532334
664,-1.3138496608,1.2868365424\H,4.2284562214,-2.3634248712,1.32842665
44\H,5.6233073207,-1.2799396761,1.3064876172\H,4.1562426275,-0.8140371
548,2.1803914648\C,4.5483148591,-1.2922787105,-1.2497193775\H,4.181241
7458,-0.7785299116,-2.139073304\H,5.6394149611,-1.2553010777,-1.256449
7846\H,4.2472885467,-2.3416046194,-1.3120133178\\Version=ES64L-G09RevD
.01\State=1-A\HF=-554.907793\RMSD=6.566e-09\RMSF=2.332e-06\Dipole=4.85
84174,-1.8459175,0.0356534\Quadrupole=-12.8718548,4.1925266,8.6793282,
-5.2609229,-0.0248993,-0.0655855\PG=C01 [X(C5H17B9N1O1)]\\@

1k

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C2H12B9O1(1-)\PIOTR\27-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl) freq(noraman, readIso)\\CB9H9-CH2OH, Cs, eclipsed
orinent\\-1,1\B,-1.6656615014,0.7934647827,-0.9204600782\B,-1.387059 57,-
1.0203183185,0.9213611436\B,-1.38705957,-1.0203183185,-0.921361143
6\B,-1.6656615014,0.7934647827,0.9204600782\B,-0.2347128122,1.39061271
65,0.\B,-0.0441648229,0.1081799354,-1.2985047041\B,0.1606384058,-1.172
2741864,0.\B,-0.0441648229,0.1081799354,1.2985047041\B,-2.6037630364,-
0.2774331973,0.\H,-3.7779119768,-0.4615371222,0.\C,0.8942627122,0.2549
427319,0.\H,-2.1786316795,1.5210707991,-1.7142858121\H,-1.6636773124,-
1.8680843196,-1.7132986332\H,-1.6636773124,-1.8680843196,1.7132986332\
H,-2.1786316795,1.5210707991,1.7142858121\H,0.105913849,2.5296586939,0
.\H,0.4627776869,0.1923926111,-2.3700347298\H,0.8038918597,-2.16674074
67,0.\H,0.4627776869,0.1923926111,2.3700347298\C,2.3657821173,0.571076
5917,0.\H,2.6048739517,1.1704268081,-0.8849926339\H,2.6048739517,1.170
4268081,0.8849926339\O,3.1453182572,-0.6289858148,0.\H,4.0747703235,-0
.3739931617,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-382.7180745\RM
SD=3.709e-09\RMSF=7.916e-06\Dipole=3.1681943,0.8521271,0.\Quadrupole=0
.2793851,-0.4692656,0.1898805,3.2905549,0.,0.\PG=CS [SG(C2H4B3O1),X(H8
B6)]\\@

1l

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H9B9Cl1(1-)\PIOTR\26-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl)\\1-CB9-1-Cl, C4v\\-1,1\B,-1.3072099253,0.,-0.010
760554\B,0.,1.3072099253,-0.010760554\B,1.3072099253,0.,-0.010760554\B
,0.,-1.3072099253,-0.010760554\B,-0.9207091648,-0.9207091648,1.4876995
094\B,-0.9207091648,0.9207091648,1.4876995094\B,0.9207091648,0.9207091
648,1.4876995094\B,0.9207091648,-0.9207091648,1.4876995094\B,0.,0.,2.5
740474046\C,0.,0.,-0.9335206481\Cl,0.,0.,-2.6907407277\H,0.,0.,3.76097
12348\H,-2.3722293893,0.,-0.5309633801\H,0.,2.3722293893,-0.5309633801
\H,2.3722293893,0.,-0.5309633801\H,0.,-2.3722293893,-0.5309633801\H,-1
.7142127945,-1.7142127945,1.8874399971\H,-1.7142127945,1.7142127945,1.
8874399971\H,1.7142127945,1.7142127945,1.8874399971\H,1.7142127945,-1.
7142127945,1.8874399971\\Version=ES64L-G09RevD.01\State=1-A1\HF=-727.7
643858\RMSD=4.868e-09\RMSF=3.600e-06\Dipole=0.,0.,-1.7237142\Quadrupol
e=3.0999286,3.0999286,-6.1998571,0.,0.,0.\PG=C04V [C4(H1B1C1Cl1),2SGV(
H2B2),2SGD(H2B2)]\\@

1m

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H15B9N3(1-)\PIOTR\29-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl)\\CB9H9-1-N=N-PhNH2, C1\\-1,1\B,-3.5664679723,2.4
477961811,-0.0098648597\B,-1.3469977773,3.8100045436,-0.0096060237\B,-
2.4562090481,3.129536739,1.2908008246\B,-2.4478739308,3.1164356988,-1.
3101971367\B,-2.4546175746,1.3596920775,-0.9160382893\B,-2.4605151604,
1.368922926,0.9140869128\B,-0.8811518397,2.3418622078,0.9160139358\B,-
0.8752816249,2.3325378504,-0.9176138269\B,-3.0266974536,4.0523196363,-
0.0161879552\H,-3.6458391649,5.0658669286,-0.0233008754\C,-1.175846672
2,1.0495534148,0.0047583744\H,-4.7330234929,2.2026263556,-0.0123592683
\H,-0.6060073676,4.7437530589,-0.0118661906\H,-2.6684326776,3.47385475
07,2.4120808882\H,-2.6529088713,3.449604698,-2.4361541618\H,-2.8233864
537,0.5209426481,-1.6697516214\H,-2.834044391,0.5376943278,1.673809534
1\H,0.0246763378,2.2962956361,1.6792193991\H,0.0352972217,2.279496752,
-1.674617045\N,-0.5121940885,-0.2140229479,0.0135125335\N,0.732044183,
-0.1510511467,0.0185278837\C,1.4173496261,-1.3865873514,0.0279032075\C
,0.8079312319,-2.6495127089,0.036639142\C,2.8122200886,-1.3152714015,0
.0315433257\C,1.574451423,-3.7957724944,0.0477093834\C,3.5871946589,-2
.4615471774,0.0429087136\C,2.9811653591,-3.7262174323,0.051618639\H,-0
.2710694507,-2.7155969827,0.0364632124\H,3.2797027826,-0.3385526554,0.
0273066924\H,1.0936706677,-4.7672603244,0.0529129368\H,4.668036133,-2.
386058098,0.0446981773\N,3.7394893376,-4.8791982855,0.0109812271\H,4.7
006507594,-4.8047470338,0.3033808034\H,3.2928022118,-5.7300063907,0.31
34904472\\Version=ES64L-G09RevD.01\State=1-A\HF=-664.1574544\RMSD=5.58
8e-09\RMSF=5.763e-07\Dipole=5.2723187,-6.7943052,0.4382208\Quadrupole=
-0.0342983,-5.6932846,5.7275829,13.9293115,2.8739798,-3.8712597\PG=C01
[X(C7H15B9N3)]\\@

1n

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C3H15B9S1\PIOTR\26-May-2022\0\
\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
F(Solvent=C6H5Cl)\\1-CB9-1-SMe2, Cs\\0,1\B,-3.0893045107,-0.7062984167
,0.\B,-0.5467174734,-0.2761670466,1.3106404698\B,-0.5467174734,-0.2761
670466,-1.3106404698\B,-0.7718032001,1.0254522659,0.\B,-0.3285049547,-
1.5651605766,0.\B,-1.8620812874,-1.4338633374,0.9206351434\B,-2.173969
6864,0.3876237201,-0.920259767\B,-1.8620812874,-1.4338633374,-0.920635
1434\B,-2.1739696864,0.3876237201,0.920259767\C,0.3664818541,-0.106202
4591,0.\S,2.1220671109,0.1097205206,0.\C,2.444685491,1.2073341358,1.39
56007728\C,2.444685491,1.2073341358,-1.3956007728\H,1.8192002714,2.093
7177248,1.3298464278\H,2.2346134719,0.6450577684,2.300697936\H,2.23461
34719,0.6450577684,-2.300697936\H,1.8192002714,2.0937177248,-1.3298464
278\H,-0.0479063271,-0.1912701829,2.3805150748\H,-0.0479063271,-0.1912
701829,-2.3805150748\H,-0.4513861497,2.1668170617,0.\H,0.374703732,-2.
5175534617,0.\H,-2.1247566527,-2.2797228708,1.7132925408\H,3.501847093

7,1.4614346508,-1.3520797939\H,3.5018470937,1.4614346508,1.3520797939\
H,-4.2566984994,-0.9057811899,0.\H,-2.7006402328,1.0995659601,-1.71317
70989\H,-2.1247566527,-2.2797228708,-1.7132925408\H,-2.7006402328,1.09
95659601,1.7131770989\\Version=ES64L-G09RevD.01\State=1-A'\HF=-745.445
0929\RMSD=4.081e-09\RMSF=2.441e-06\Dipole=5.9345197,2.062557,0.\Quadru
pole=1.4423738,-2.0995423,0.6571685,4.1906492,0.,0.\PG=CS [SG(C1H3B3S1
),X(C2H12B6)]\\@

1o

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H14B9N1\PIOTR\26-May-2022\0\
\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
F(Solvent=C6H5Cl) freq(noraman, readIso)\\1-CB9-2-Pyridine, C1, re-sta
rts at B3LYP/6-31G(d,p) geo\\0,1\B,-0.9229401836,0.9402073203,2.589283
0617\B,0.8802348884,-0.9405756265,2.647695329\B,-0.9644089001,-0.89971
33544,2.588564253\B,0.9216706932,0.8978736813,2.6484118881\B,0.0595583
53,1.3098978265,1.1281172132\B,-1.2683456617,0.0281488709,1.0861646185
\B,0.0004653953,-1.3121544406,1.1270941471\B,1.3304287414,-0.030450666
,1.1673583925\B,-0.0571100553,-0.0001711921,3.7075641031\C,0.060490030
4,-0.0014459428,0.1806571052\C,0.0957574297,-0.0016691738,-1.281241548
1\C,-1.2090854897,0.0285415439,-3.2817255484\C,1.1619567109,-0.0248702
963,-3.4377344807\N,-1.0843119576,0.0252027416,-1.9411046154\C,1.25222
3933,-0.0274471354,-2.0568541604\C,-0.0841845514,0.0034798759,-4.06654
21257\H,-1.7117714193,1.7488686025,2.9608949095\H,1.6412267519,-1.7486
842603,3.0743547038\H,-1.7888748681,-1.6723068278,2.9595606782\H,1.718
2879647,1.6705454153,3.0756889672\H,0.0965567809,2.3741272529,0.609078
1356\H,-2.332183518,0.052333922,0.5532565462\H,-0.0105110794,-2.376565
5114,0.6072256398\H,2.4206260352,-0.0548401791,0.7049901302\H,-0.09585
68736,0.0002398926,4.8916845449\H,-2.2157411532,0.0513956557,-3.670024
6028\H,2.0651280545,-0.0450059882,-4.0327402378\H,-1.9230989485,0.0438
923689,-1.3671875231\H,2.2090145311,-0.049219708,-1.5595404313\H,-0.17
75684985,0.0060071874,-5.1417535775\\Version=ES64L-G09RevD.01\State=1-
A\HF=-515.7838317\RMSD=8.227e-09\RMSF=1.948e-06\Dipole=-0.6328919,0.01
72653,-7.6560792\Quadrupole=4.2027127,-7.3324387,3.129726,-0.2612492,2
.4995741,-0.0604688\PG=C01 [X(C6H14B9N1)]\\@

1p

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H13B9I1(1-)\PIOTR\28-May-202
2\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl)\\1-CB9 1-Ph-10-I, C2v\\-1,1\B,0.,1.3072962429,-0
.6039325781\B,0.,-1.3072962429,-0.6039325781\B,1.3056588472,0.,-0.6038
040232\B,-1.3056588472,0.,-0.6038040232\B,-0.917423311,0.9202399839,0.
8953191819\B,0.917423311,0.9202399839,0.8953191819\B,0.917423311,-0.92
02399839,0.8953191819\B,-0.917423311,-0.9202399839,0.8953191819\B,0.,0
.,-1.6700461699\C,0.,0.,1.8457060266\C,0.,0.,3.3319213409\C,0.,1.20050
50081,5.4397669924\C,0.,-1.2005050081,5.4397669924\C,0.,1.1994862885,4
.04966443\C,0.,-1.1994862885,4.04966443\C,0.,0.,6.1425073845\H,0.,2.42
36442419,-1.0151133343\H,0.,-2.4236442419,-1.0151133343\H,2.4240521808
,0.,-1.0090287363\H,-2.4240521808,0.,-1.0090287363\H,-1.6800471071,1.6
754353466,1.3992174648\H,1.6800471071,1.6754353466,1.3992174648\H,1.68
00471071,-1.6754353466,1.3992174648\H,-1.6800471071,-1.6754353466,1.39
92174648\H,0.,2.142684814,5.9742843177\H,0.,-2.142684814,5.9742843177\
H,0.,2.1390015354,3.512106848\H,0.,-2.1390015354,3.512106848\H,0.,0.,7
.2253725292\I,0.,0.,-3.8632166379\\Version=ES64L-G09RevD.01\State=1-A1
\HF=-796.5196658\RMSD=8.718e-09\RMSF=7.574e-07\Dipole=0.,0.,2.3208486\
Quadrupole=1.0576076,6.7873784,-7.844986,0.,0.,0.\PG=C02V [C2(H1C1C1C1
B1I1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\@

1q

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H8B9I1N2\PIOTR\28-May-2022\0
\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SC
RF(Solvent=C6H5Cl)\\1-CB8-1-N2, C4v\\0,1\B,0.,-1.3347471347,-2.0306297
046\B,-1.3347471347,0.,-2.0306297046\B,0.,1.3347471347,-2.0306297046\B
,1.3347471347,0.,-2.0306297046\B,0.9289548242,-0.9289548242,-0.5577817

339\B,-0.9289548242,-0.9289548242,-0.5577817339\B,-0.9289548242,0.9289
548242,-0.5577817339\B,0.9289548242,0.9289548242,-0.5577817339\B,0.,0.
,0.5199130822\C,0.,0.,-2.9517218909\N,0.,0.,-4.3036225368\N,0.,0.,-5.4
059615406\H,0.,-2.3813690678,-2.5742912056\H,-2.3813690678,0.,-2.57429
12056\H,0.,2.3813690678,-2.5742912056\H,2.3813690678,0.,-2.5742912056\
H,1.7135591676,-1.7135591676,-0.144484477\H,-1.7135591676,-1.713559167
6,-0.144484477\H,-1.7135591676,1.7135591676,-0.144484477\H,1.713559167
6,1.7135591676,-0.144484477\I,0.,0.,2.6761540013\\Version=ES64L-G09Rev
D.01\State=1-A1\HF=-674.1030955\RMSD=9.613e-09\RMSF=6.962e-07\Dipole=0
.,0.,-3.9691643\Quadrupole=-7.9704019,-7.9704019,15.9408037,0.,0.,0.\P
G=C04V [C4(N1N1C1B1I1),2SGV(H2B2),2SGD(H2B2)]\\@

1r

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C2H9B9N2O2\PIOTR\28-May-2022\0
\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SC
RF(Solvent=C6H5Cl) freq(noraman, readIso)\\N2-CB9H8-COOMe, Cs\\0,1\B,1
.717171783,-0.2027877501,0.\B,-0.5320343541,-1.6137701471,0.\B,0.58955
26652,-0.9026120345,1.3255443744\B,0.5895526652,-0.9026120345,-1.32554
43744\B,0.5898052766,0.8526285984,-0.9236503327\B,0.5898052766,0.85262
85984,0.9236503327\B,-0.9903367135,-0.1384089387,0.9244852797\B,-0.990
3367135,-0.1384089387,-0.9244852797\B,1.1342123518,-1.771646225,0.\N,1
.9115613145,-3.020514349,0.\N,2.4883374972,-3.9528984968,0.\C,-0.69123
6371,1.1395164618,0.\C,-1.4442770367,2.4267230408,0.\H,-3.1996774,3.11
05226484,0.\O,-0.929893555,3.5164120042,0.\O,-2.7733122073,2.237452674
9,0.\H,2.8822431676,0.0075911844,0.\H,-1.2293757492,-2.5706500131,0.\H
,0.8195928716,-1.270412468,2.4271912271\H,0.8195928716,-1.270412468,-2
.4271912271\H,0.9534007493,1.6827555283,-1.6794102061\H,0.9534007493,1
.6827555283,1.6794102061\H,-1.893811092,-0.1089251685,1.6832824532\H,-
1.893811092,-0.1089251685,-1.6832824532\\Version=ES64L-G09RevD.01\Stat
e=1-A'\HF=-565.6001205\RMSD=4.772e-09\RMSF=1.168e-05\Dipole=0.4156866,
-2.002157,0.\Quadrupole=3.6966659,1.4872907,-5.1839566,-12.7102254,0.,
0.\PG=CS [SG(C2H3B3N2O2),X(H6B6)]\\@

1s

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H14B9N1O2\PIOTR\28-May-2022\
0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S
CRF(Solvent=C6H5Cl)\\PyrCB9COOH   C1\\0,1\B,-1.7793159726,-0.3312457884,
-1.2801687656\B,-1.7794996439,-1.2691412132,0.3054374401\B,-1.69478651
7,0.331234184,1.2490309895\B,-1.6943979198,1.2687164894,-0.3352158924\
B,-0.2480713838,0.6079309168,-1.176851079\B,-0.3016681348,-1.187740675
4,-0.7138735505\B,-0.2484895823,-0.7245195588,1.0784599325\B,-0.182845
2606,1.0701192453,0.6148492109\B,0.8059882468,-0.0998970042,-0.0735579
868\N,2.3307901012,-0.1596357809,-0.1080472562\C,3.0464363615,0.945483
5342,-0.4031723421\C,4.4248193117,0.9211307801,-0.4415997389\C,5.08992
74617,-0.2678681828,-0.169992682\C,4.3466004403,-1.4016231779,0.133302
5772\C,2.9702410966,-1.317864664,0.1568047682\C,-2.666964215,0.0364637
209,0.0061784318\C,-4.1479049537,0.1292442367,0.0637830329\O,-4.752638
6098,-0.8944527959,-0.5681840278\O,-4.7646251887,1.0118245215,0.609508
6066\H,-2.3153967347,-0.57176629,-2.3060606524\H,-2.3196326934,-2.2817
946189,0.5898598944\H,-2.1686616174,0.6116662086,2.2949766956\H,-2.170
6501035,2.3193386079,-0.5947274398\H,0.1766783325,1.1533927286,-2.1437
338847\H,0.0791868844,-2.15599175,-1.2886818622\H,0.176165224,-1.30353
99608,2.0256610949\H,0.2978618819,2.0046423007,1.1700597997\H,2.475732
6484,1.8388032168,-0.6043771933\H,4.9622805829,1.8267561867,-0.6816882
573\H,6.1702934857,-0.3102200755,-0.1941419693\H,4.8217534302,-2.34687
67702,0.3509816823\H,2.3409457544,-2.164010344,0.385349247\H,-5.711640
7132,-0.7642222276,-0.4868688238\\Version=ES64L-G09RevD.01\State=1-A\H
F=-704.4751241\RMSD=5.795e-09\RMSF=4.524e-06\Dipole=5.4647593,-0.80577
36,-0.4897677\Quadrupole=26.0840477,-9.8724629,-16.2115848,5.5272991,3
.2138448,-3.8992314\PG=C01 [X(C7H14B9N1O2)]\\@

1t

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H19B9O2S1\PIOTR\28-May-2022\

0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S
CRF(Solvent=C6H5Cl) freq(noraman, readIso)\\10-ThiaCB9-1-COOH Cs\\0,1\
B,2.0496566306,0.9206473927,1.226067885\B,2.0496566306,-0.9206473927,1
.226067885\B,2.3309810815,-0.9175833923,-0.6174949545\B,2.3309810815,0
.9175833923,-0.6174949545\B,0.7129138825,1.3101482077,0.0784358472\B,0
.7129138825,-1.3101482077,0.0784358472\B,0.5149854803,0.,1.3817513628\
B,0.9110406162,0.,-1.2181692521\B,-0.3233846813,0.,-0.0734158175\S,-2.
1637443432,0.,-0.4167106597\C,-2.836545187,1.3919792298,0.5635392289\C
,-2.836545187,-1.3919792298,0.5635392289\C,-4.3544246549,1.2786943881,
0.6695291857\C,-4.3544246549,-1.2786943881,0.6695291857\C,-4.818604408
5,0.,1.3726941197\C,3.1092696211,0.,0.4464744265\C,4.5841278573,0.,0.6
328060625\O,4.9367928959,0.,1.9318355819\O,5.3933410855,0.,-0.26229534
49\H,2.4347607288,1.6834177389,2.0428931326\H,2.4347607288,-1.68341773
89,2.0428931326\H,2.9482782706,-1.6765919751,-1.2807726411\H,2.9482782
706,1.6765919751,-1.2807726411\H,0.309670435,2.4257041585,0.0182276506
\H,0.309670435,-2.4257041585,0.0182276506\H,-0.0679134991,0.,2.4177294
276\H,0.6519511515,0.,-2.3768801295\H,-4.7049337509,-2.153133405,1.222
8498631\H,-4.7049337509,2.153133405,1.2228498631\H,-2.5252458628,2.291
8847729,0.0367014813\H,-2.5252458628,-2.2918847729,0.0367014813\H,-2.3
507486329,1.3661199293,1.538578155\H,-2.3507486329,-1.3661199293,1.538
578155\H,-4.7975434897,1.3424001047,-0.3282230288\H,-4.7975434897,-1.3
424001047,-0.3282230288\H,-5.9084020909,0.,1.431153536\H,5.9071716811,
0.,1.9734243885\H,-4.4501073206,0.,2.4035737012\\Version=ES64L-G09RevD
.01\State=1-A'\HF=-1050.926878\RMSD=8.263e-09\RMSF=2.108e-06\Dipole=-4
.9913318,0.,1.1520844\Quadrupole=12.0243195,-2.8598618,-9.1644576,0.,7
.8507128,0.\PG=CS [SG(C3H5B3O2S1),X(C4H14B6)]\\@

1u

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C16H24B9I1O1\PIOTR\13-Jan-2023
\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl)\\10-PhI-CB9H8-1-CH2CH2-PhOMe, C1\\0,1\B,2.4063466
954,0.888340431,1.2364911108\B,2.2117734649,-0.7700143664,-0.798670173
4\B,2.3113997628,-0.9691471671,1.044786607\B,2.300243285,1.0852530549,
-0.6055766889\B,0.8725840952,1.4137680088,0.4376016065\B,0.8869672721,
-0.0158506415,1.5961540655\B,0.7442045479,-1.1683782977,0.1712479736\B
,0.743846992,0.2638737161,-0.9858544341\B,3.3311889535,0.0132781844,0.
1608562699\C,-0.1286586171,0.1612566072,0.3632448135\H,2.8986326497,1.
5678718772,2.0770055936\H,2.5448607276,-1.4853449248,-1.68724902\H,2.7
276727451,-1.852429765,1.721261393\H,2.7164860477,1.9288576554,-1.3312
54031\H,0.4184577056,2.4985201455,0.5831754528\H,0.4404995788,-0.10739
07111,2.6900052396\H,0.1891114199,-2.2125262298,0.0914992531\H,0.20252
39632,0.3969849694,-2.0289935936\C,-3.923632147,0.1714049619,-0.572765
4148\C,-4.6231615444,1.3814029269,-0.5045784608\C,-4.6528750768,-1.001
2558178,-0.3971137536\C,-5.9872851129,1.4180173715,-0.2681181362\C,-6.
0261696934,-0.9875573756,-0.1580012726\C,-6.7011976274,0.2299332616,-0
.0911286117\C,-1.637707787,0.2170780888,0.5170549121\C,-2.4315455215,0
.1440353199,-0.7984742852\O,-8.0403134564,0.361592143,0.1332417937\C,-
8.8160370942,-0.8159017934,0.317895847\H,-4.089311778,2.3146263101,-0.
645219454\H,-4.1453524786,-1.9579528243,-0.4512514499\H,-6.5199080618,
2.3594797788,-0.2225665328\H,-6.5507170221,-1.9234541795,-0.0320734023
\H,-1.9512210617,-0.6065872322,1.162371873\H,-1.9044173977,1.137492186
9,1.0413064123\H,-2.1558471851,-0.7691965649,-1.3310254274\H,-2.142432
8632,0.9798398871,-1.43872614\H,-8.4772184955,-1.3835079313,1.18870524
29\H,-9.8368534306,-0.4794275491,0.4820703676\H,-8.784024588,-1.456994
0771,-0.5671600802\I,5.5294762105,-0.0934493294,-0.0619199384\C,6.1823
086213,0.0546813476,1.959849287\C,6.2584738137,-1.1031606226,2.7188098
19\C,6.527647618,1.3034444728,2.4535902192\C,6.6969301595,-0.994786563
2,4.0354030359\H,5.9835421385,-2.0646858683,2.3099425332\C,6.965539206
6,1.3877743384,3.7722873552\H,6.4573909669,2.1909428415,1.8413788808\C
,7.0491029411,0.2443608571,4.5588981156\H,6.760233146,-1.8851868464,4.
6469836813\H,7.237564124,2.3529827015,4.1788504572\H,7.3890738779,0.31
9226003,5.5834450389\\Version=ES64L-G09RevD.01\State=1-A\HF=-1221.2658
389\RMSD=1.931e-09\RMSF=2.482e-06\Dipole=3.4397209,-0.6007605,1.300650

5\Quadrupole=30.8840058,-15.9326111,-14.9513947,11.3376492,10.3597353,
0.1983261\PG=C01 [X(C16H24B9I1O1)]\\@

1v

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C10H19B9I1O1(1-)\PIOTR\29-May-
2022\0\\#P B3LYP/Def2TZVP FOpt(tight, RCFC) geom(noangle, nodistance)
fcheck #P SCRF(Solvent=C6H5Cl) guess=check\\10-I-CB9H8-1-CH2CH2-PhOMe,
C1\\-1,1\B,-1.5195343513,2.5488373203,0.1093251412\B,1.070210978,2.25
27759262,-0.0617566846\B,-0.1444542249,2.3505688588,1.3247268562\B,-0.
30820652,2.4519467747,-1.2796542263\B,-1.3609200094,1.0490468655,-0.88
111292\B,-1.248104784,0.9784289828,0.9464519005\B,0.5711868127,0.77005
82588,0.8264528076\B,0.4549784741,0.8418525136,-1.003136645\B,-0.10167
35215,3.4590299386,0.0571914778\C,-0.5044592212,-0.03256691,-0.0546185
356\H,-2.581475745,3.0789098049,0.1967808839\H,2.2248049443,2.53471929
43,-0.124393474\H,-0.0287252636,2.7085490512,2.4538510269\H,-0.3290537
659,2.9026568598,-2.381003243\H,-2.2206388485,0.6587065767,-1.60121876
2\H,-2.0107388791,0.5290180028,1.7380275048\H,1.3120864633,0.154156478
4,1.5207997935\H,1.1095609561,0.3047131511,-1.832090844\C,0.0279787274
,-3.8326899461,-0.8044431327\C,-0.8551682319,-4.482097523,-1.674215131
5\C,0.6525497919,-4.6077930386,0.1688518256\C,-1.1032367018,-5.8415219
568,-1.5751370066\C,0.4177919084,-5.9770797407,0.2865874058\C,-0.46742
88996,-6.6012386422,-0.5901713447\C,-0.7200983869,-1.5337733928,-0.044
780397\C,0.2689609201,-2.3458853436,-0.8985163811\O,-0.769760537,-7.93
26417263,-0.5689199619\C,-0.1415851861,-8.7538924037,0.4065682748\H,-1
.3553519402,-3.9120307778,-2.4491407062\H,1.3476916783,-4.1395381855,0
.8568126957\H,-1.7851381455,-6.3342878879,-2.2566794412\H,0.9294746943
,-6.5376258136,1.05539368\H,-0.6592882348,-1.8867817673,0.9878935464\H
,-1.7371934918,-1.7496328139,-0.3816302336\H,1.2877648483,-2.118173480
4,-0.5761660001\H,0.1921831361,-2.0268033798,-1.939992982\H,-0.3951355
2,-8.433912848,1.4209134582\H,-0.520680559,-9.7595865228,0.2412229552\
H,0.9454374086,-8.7528045217,0.2882736127\I,0.1575025972,5.6380748039,
0.1272200062\\Version=ES64L-G09RevD.01\State=1-A\HF=-989.7443839\RMSD=
1.920e-09\RMSF=1.586e-06\Dipole=0.2843482,-6.0151161,0.0641702\Quadrup
ole=10.2533099,-21.9812389,11.727929,-5.5092885,2.2700472,-10.8272529\
PG=C01 [X(C10H19B9I1O1)]\\@

1w

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H9B9N2\PIOTR\28-May-2022\0\\
#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF
(Solvent=C6H5Cl) freq(noraman, readIso)\\1-CB9-10-B2, C4v\\0,1\B,-1.32
51243334,0.,-0.0861763691\B,0.,1.3251243334,-0.0861763691\B,1.32512433
34,0.,-0.0861763691\B,0.,-1.3251243334,-0.0861763691\B,-0.9260112101,-
0.9260112101,1.4085175588\B,-0.9260112101,0.9260112101,1.4085175588\B,
0.9260112101,0.9260112101,1.4085175588\B,0.9260112101,-0.9260112101,1.
4085175588\C,0.,0.,2.3238889732\B,0.,0.,-1.111144137\N,0.,0.,-2.579695
2869\N,0.,0.,-3.6767706249\H,0.,0.,3.4002370447\H,-2.4261919036,0.,-0.
5238310467\H,0.,2.4261919036,-0.5238310467\H,2.4261919036,0.,-0.523831
0467\H,0.,-2.4261919036,-0.5238310467\H,-1.6833398909,-1.6833398909,1.
9091238258\H,-1.6833398909,1.6833398909,1.9091238258\H,1.6833398909,1.
6833398909,1.9091238258\H,1.6833398909,-1.6833398909,1.9091238258\\Ver
sion=ES64L-G09RevD.01\State=1-A1\HF=-376.9483315\RMSD=2.463e-09\RMSF=3
.089e-06\Dipole=0.,0.,-1.2731957\Quadrupole=-4.559658,-4.559658,9.1193
16,0.,0.,0.\PG=C04V [C4(H1C1B1N1N1),2SGV(H2B2),2SGD(H2B2)]\\@

1x

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H14B9N1\PIOTR\05-Apr-2023\0\
\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
F(Solvent=C6H5Cl) freq(NoRaman)\\10-CB9-1-Pyridine, C2v\\0,1\B,-1.3056
029941,0.,-2.4529090059\B,1.3056029941,0.,-2.4529090059\B,0.,1.3042732
213,-2.4528887575\B,0.,-1.3042732213,-2.4528887575\B,-0.9267186632,-0.
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,0.,0.,0.\PG=C02V [C2(H1C1B1N1C1H1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\@

1y

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C3H15B9N2\PIOTR\30-May-2022\0\
\#P B3LYP/Def2TZVP FOpt(tight, RCFC) geom(noangle, nodistance) fcheck
#P SCRF(Solvent=C6H5Cl)\\CB9-10-acemtamidinium, C1\\0,1\B,-2.048976335
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702371,-0.0171497833\C,-3.1506343853,0.2629170151,0.0167519435\H,-2.38
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\PG=C01 [X(C3H15B9N2)]\\@

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