DFT analysis: correlation of epinephrine HOMO-LUMO, refractive index, optical electronegativity, and electrical conductivity with Substituted Halogens (F, Cl, Br)

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Input File For Title Compounds, And Optimized Cartesian Coordinates (Å) Of Structures

The Gaussian 09W software suite was used to look at the structure of the norepinephrine (NEP) molecule using different halogens, which were named NEP, NEP-Br, NEP-Cl, and NEP-F. A useful way to study molecular structure is through the density-functional theory (DFT)/ default spin, and singlet spin. Based on the B3LYP level of theory, and 6- 311G(d, p) basis set, the NEP molecule was optimized by using the DFT methodology.

Table S1. Input File for NEP opt b3lyp/6-311g(d,p) geom=connectivity

NEP	X	Y	Z	NEP-Br	X	Y	Z
O	2.96738	1.88707	0.49698	O	2.96738	1.88707	0.49698
O	4.13624	-0.55469	0.53391	O	4.13624	-0.55469	0.53391
O	-1.73572	1.3003	-1.15888	O	-1.73572	1.3003	-1.15888
N	-3.73088	-0.15278	0.03705	N	-3.73088	-0.15278	0.03705
C	0.05014	-0.22449	-0.51516	C	0.05014	-0.22449	-0.51516
C	2.17211	0.78693	0.16579	C	2.17211	0.78693	0.16579
C	2.78404	-0.48817	0.18211	C	2.78404	-0.48817	0.18211
C	0.81668	0.90823	-0.17954	C	0.81668	0.90823	-0.17954
C	-1.42691	-0.08522	-0.84117	C	-1.42691	-0.08522	-0.84117
C	0.66411	-1.4906	-0.51141	C	0.66411	-1.4906	-0.51141
				C	2.02171	-1.61818	-0.16079
				C	-2.33057	-0.51814	0.34715
				C	-4.63973	-0.03396	1.19483
				H	2.46125	2.72251	0.42496
				H	4.46763	-1.47561	0.50044
				H	-2.70259	1.40413	-0.97276
				H	-4.12425	-0.74339	-0.69776
				H	0.33743	1.88342	-0.21784
				H	-1.66693	-0.72187	-1.71182
				H	2.49353	-2.60034	-0.16093
				H	-2.18816	-1.59175	0.56263

C	2.02171	-1.61818	-0.16079	H	-2.02585	0.04391	1.23885
C	-2.33057	-0.51814	0.34715	H	-5.63999	0.25063	0.84781
C	-4.63973	-0.03396	1.19483	H	-4.72985	-0.96237	1.78824
H	2.46125	2.72251	0.42496	H	-4.27794	0.75814	1.86128
H	4.46763	-1.47561	0.50044	Br	-0.32776	-3.04814	-0.99961
H	-2.70259	1.40413	-0.97276				
H	-4.12425	-0.74339	-0.69776				
H	0.33743	1.88342	-0.21784				
H	-1.66693	-0.72187	-1.71182				
H	0.09916	-2.37775	-0.78948				
H	2.49353	-2.60034	-0.16093				
H	-2.18816	-1.59175	0.56263				
H	-2.02585	0.04391	1.23885				
H	-5.63999	0.25063	0.84781				
H	-4.72985	-0.96237	1.78824				
H	-4.27794	0.75814	1.86128				

NEP-Cl	X	Y	Z	NEP-F	X	Y	Z
O	2.96738	1.88707	0.49698	O	2.96738	1.88707	0.49698
O	4.13624	-0.55469	0.53391	O	4.13624	-0.55469	0.53391
O	-1.73572	1.3003	-1.15888	O	-1.73572	1.3003	-1.15888
N	-3.73088	-0.15278	0.03705	N	-3.73088	-0.15278	0.03705
C	0.05014	-0.22449	-0.51516	C	0.05014	-0.22449	-0.51516
C	2.17211	0.78693	0.16579	C	2.17211	0.78693	0.16579
C	2.78404	-0.48817	0.18211	C	2.78404	-0.48817	0.18211
C	0.81668	0.90823	-0.17954	C	0.81668	0.90823	-0.17954
C	-1.42691	-0.08522	-0.84117	C	-1.42691	-0.08522	-0.84117
C	0.66411	-1.4906	-0.51141	C	0.66411	-1.4906	-0.51141
C	2.02171	-1.61818	-0.16079	C	2.02171	-1.61818	-0.16079
C	-2.33057	-0.51814	0.34715	C	-2.33057	-0.51814	0.34715
C	-4.63973	-0.03396	1.19483	C	-4.63973	-0.03396	1.19483
H	2.46125	2.72251	0.42496	H	2.46125	2.72251	0.42496
H	4.46763	-1.47561	0.50044	H	4.46763	-1.47561	0.50044
H	-2.70259	1.40413	-0.97276	H	-2.70259	1.40413	-0.97276
H	-4.12425	-0.74339	-0.69776	H	-4.12425	-0.74339	-0.69776
H	0.33743	1.88342	-0.21784	H	0.33743	1.88342	-0.21784
H	-1.66693	-0.72187	-1.71182	H	-1.66693	-0.72187	-1.71182
H	2.49353	-2.60034	-0.16093	H	2.49353	-2.60034	-0.16093

H	**-2.18816**	**-1.59175**	**0.56263**	**H**	**-2.18816**	**-1.59175**	**0.56263**
H	**-2.02585**	**0.04391**	**1.23885**	**H**	**-2.02585**	**0.04391**	**1.23885**
H	**-5.63999**	**0.25063**	**0.84781**	**H**	**-5.63999**	**0.25063**	**0.84781**
H	**-4.72985**	**-0.96237**	**1.78824**	**H**	**-4.72985**	**-0.96237**	**1.78824**
H	**-4.27794**	**0.75814**	**1.86128**	**H**	**-4.27794**	**0.75814**	**1.86128**
Cl	**-0.24987**	**-2.92582**	**-0.96127**	**F**	**-0.03695**	**-2.59148**	**-0.85647**

Optimized Cartesian Coordinates (Å)

B3LYP/6-311G(d,p),

NEP/ SCF: -631.359510443 a.u		**NEP-Br/ SCF -3204.89316714 a.u**	
O	**2.94466 1.84812 0.49686**	**O**	**2.96738 1.88707 0.49698**
O	**4.07687 -0.545690.53438**	**O**	**4.13624 -0.554690.53391**
O	**-1.707661.28706 -1.17156**	**O**	**-1.735721.3003 -1.15888**
N	**-3.70428-0.118320.03211**	**N**	**-3.73088-0.152770.03705**
C	**0.05004 -0.21221-0.51087**	**C**	**0.05014 -0.22449-0.51516**
C	**2.15435 0.78014 0.16809**	**C**	**2.17211 0.78693 0.16579**
C	**2.75354 -0.484190.1863**	**C**	**2.78404 -0.488170.18211**
C	**0.81462 0.90631 -0.17529**	**C**	**0.81668 0.90823 -0.17954**
C	**-1.41665-0.06693-0.84092**	**C**	**-1.42691-0.08522-0.84117**
C	**0.65342 -1.46799-0.50404**	**C**	**0.66411 -1.4906 -0.51141**
C	**1.99579 -1.59867-0.15285**	**C**	**2.02171 -1.61818-0.16079**
C	**-2.31987-0.478850.33898**	**C**	**-2.33057-0.518140.34715**
C	**-4.59381-0.053911.18775**	**C**	**-4.63973-0.033951.19483**
H	**2.40208 2.63869 0.41047**	**H**	**2.46124 2.72251 0.42496**
H	**4.34363 -1.469140.48568**	**H**	**4.46763 -1.475610.50044**
H	**-2.656931.33987 -0.97001**	**H**	**-2.702591.40413 -0.97276**
H	**-4.08477-0.74494-0.6679**	**H**	**-4.12425-0.74338-0.69776**
H	**0.34622 1.88285 -0.20819**	**H**	**0.33743 1.88342 -0.21784**
H	**-1.65442-0.70641-1.70467**	**H**	**-1.66693-0.72187-1.71182**
H	**0.08805 -2.35075-0.78205**	**H**	**2.49353 -2.60034-0.16093**
H	**2.4648 -2.5777 -0.15002**	**H**	**-2.18816-1.591750.56263**
H	**-2.18057-1.545920.56879**	**H**	**-2.025850.04391 1.23885**
H	**-2.017 0.09387 1.21951**	**H**	**-5.639990.25063 0.84781**
H	**-5.601750.19659 0.85009**	**H**	**-4.72985-0.962371.78824**
H	**-4.64405-0.988071.76902**	**H**	**-4.277940.75814 1.86128**
H	**-4.254290.74219 1.85485**	**Br**	**-0.32776-3.04814-0.99961**

NEP-Cl/ SCF: -1090.97340679 a.u		**NEP-F/ SCF -730.616622194a.u**	
O	**2.96738 1.88707 0.49698**	**O**	**2.96738 1.88707 0.49698**
O	**4.13624 -0.554690.53391**	**O**	**4.13624 -0.554690.53391**
O	**-1.735721.3003 -1.15888**	**O**	**-1.735721.3003 -1.15888**
N	**-3.73088-0.152770.03705**	**N**	**-3.73088-0.152770.03705**
C	**0.05014 -0.22449-0.51516**	**C**	**0.05014 -0.22449-0.51516**
C	**2.17211 0.78693 0.16579**	**C**	**2.17211 0.78693 0.16579**
C	**2.78404 -0.488170.18211**	**C**	**2.78404 -0.488170.18211**
C	**0.81668 0.90823 -0.17954**	**C**	**0.81668 0.90823 -0.17954**
C	**-1.42691-0.08522-0.84117**	**C**	**-1.42691-0.08522-0.84117**
C	**0.66411 -1.4906 -0.51141**	**C**	**0.66411 -1.4906 -0.51141**
C	**2.02171 -1.61818-0.16079**	**C**	**2.02171 -1.61818-0.16079**
C	**-2.33057-0.518140.34715**	**C**	**-2.33057-0.518140.34715**
C	**-4.63973-0.033951.19483**	**C**	**-4.63973-0.033951.19483**
H	**2.46124 2.72251 0.42496**	**H**	**2.46124 2.72251 0.42496**

H	**4.46763 -1.475610.50044**	**H**	**4.46763 -1.475610.50044**
H	**-2.702591.40413 -0.97276**	**H**	**-2.702591.40413 -0.97276**
H	**-4.12425-0.74338-0.69776**	**H**	**-4.12425-0.74338-0.69776**
H	**0.33743 1.88342 -0.21784**	**H**	**0.33743 1.88342 -0.21784**
H	**-1.66693-0.72187-1.71182**	**H**	**-1.66693-0.72187-1.71182**
H	**2.49353 -2.60034-0.16093**	**H**	**2.49353 -2.60034-0.16093**
H	**-2.18816-1.591750.56263**	**H**	**-2.18816-1.591750.56263**
H	**-2.025850.04391 1.23885**	**H**	**-2.025850.04391 1.23885**
H	**-5.639990.25063 0.84781**	**H**	**-5.639990.25063 0.84781**
H	**-4.72985-0.962371.78824**	**H**	**-4.72985-0.962371.78824**
H	**-4.277940.75814 1.86128**	**H**	**-4.277940.75814 1.86128**
Cl	**-0.24987-2.92582-0.96127**	**F**	**-0.03695-2.59148-0.85647**