Supporting Information

Ca-, Li-, and Cu-Salicylatoborates for Potential Applications in Neutron Capture Therapy: A Computational Method for the Preliminary Discrimination of the More Promising Compounds

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Section S1

Table S1. Crystal data and structure refinements for CaSB, CuSB, and LiSB.

	CaSB	**CuSB**	**LiSB**
Empirical formula	$C_{28}H_{36}B_2CaO_{22}$	$C_{28}H_{16}B_2CuO_{12}$	$C_{14}H_{10}BLiO_7$
Formula weight	786.27	629.57	307.97
Temperature/ K	293(2)	293(2)	293(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	P2/n	$P2_1/c$
a/ Å	9.8996(3)	12.6250(2)	10.720(5)
b/ Å	12.4244(3)	6.52160(10)	8.347(4)
c/ Å	28.8806(8)	16.7556(2)	15.446(6)
β/ °	93.556(2)	108.988(1)	101.52(4)
Volume/ $Å^3$	3545.4(2)	1304.51(3)	1354.3(10)
Z	4	2	4
ρ_{calc}/ g/cm^3	1.473	1.603	1.510
μ/ mm^{-1}	2.325	1.798	1.016
F(000)	1640.0	638.0	632.0
Crystal size/ mm^3	0.229 × 0.196 × 0.054	0.244 × 0.076 × 0.034	0.103 × 0.055 × 0.02
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/ °	7.748 to 133.628	7.686 to 133.854	8.418 to 100.87
Index ranges	$-11 \le h \le 11$ $-14 \le k \le 14$ $-33 \le l \le 34$	$-15 \le h \le 14$ $-7 \le k \le 7$ $-19 \le l \le 19$	$-10 \le h \le 10$ $-7 \le k \le 8$ $-15 \le l \le 10$
Reflections collected	49769	12674	6161
Independent reflections	6194	2317	1417
R_{int}	0.0617	0.0235	0.1003
R_{sigma}	0.0320	0.0157	0.0827
Data/restraints/parameters	6194/0/501	2317/0/195	1417/0/211
Goodness-of-fit on F^2	1.064	1.051	1.036
Final R indexes [I>=2σ (I)]	$R_1 = 0.1031$ $wR_2 = 0.3319$	$R_1 = 0.0300$ $wR_2 = 0.0796$	$R_1 = 0.0604$ $wR_2 = 0.1247$
Final R indexes [all data]	$R_1 = 0.1285$ $wR_2 = 0.3803$	$R_1 = 0.0320$ $wR_2 = 0.0815$	$R_1 = 0.1210$ $wR_2 = 0.1576$
Largest diff. peak/hole /$eÅ^{-3}$	0.84/-1.95	0.32/-0.33	0.20/-0.17

Table S2. Bond Angles for CaSB.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1X	Ca1A	O2X	176.1(2)	C1B	O2B	B1AB	125.1(4)	C7A	C2A	C1A	120.7(4)
O1X	Ca1A	O4X	90.81(18)	C3B	O3B	B1AB	122.9(4)	O3A	C3A	C2A	121.9(4)
O1X	Ca1A	O5X	88.82(17)	O1B	C1B	O2B	119.3(4)	O3A	C3A	C4A	118.0(4)
O3X	Ca1A	O1X	91.79(18)	O1B	C1B	C2B	123.0(4)	C2A	C3A	C4A	120.1(4)
O3X	Ca1A	O2X	91.25(18)	O2B	C1B	C2B	117.7(3)	C5A	C4A	C3A	119.3(5)
O3X	Ca1A	O4X	90.62(18)	C3B	C2B	C1B	119.6(4)	C4A	C5A	C6A	120.7(5)
O3X	Ca1A	O5X	178.0(2)	C3B	C2B	C7B	119.5(4)	C7A	C6A	C5A	120.0(5)
O3X	Ca1A	O6X	91.15(16)	C7B	C2B	C1B	120.9(4)	C6A	C7A	C2A	120.5(5)
O4X	Ca1A	O2X	86.69(16)	O3B	C3B	C2B	121.5(4)	C7D	C2D	C1D	120.6(4)
O5X	Ca1A	O2X	88.07(17)	O3B	C3B	C4B	119.2(4)	O3D	C3D	C2D	122.1(4)
O5X	Ca1A	O4X	87.46(15)	C2B	C3B	C4B	119.3(5)	O3D	C3D	C4D	118.1(4)
O6X	Ca1A	O1X	90.09(18)	C5B	C4B	C3B	120.2(5)	C2D	C3D	C4D	119.8(4)
O6X	Ca1A	O2X	92.32(18)	C4B	C5B	C6B	120.8(5)	C5D	C4D	C3D	120.3(4)
O6X	Ca1A	O4X	178.0(2)	C7B	C6B	C5B	119.6(5)	C4D	C5D	C6D	120.8(4)
O6X	Ca1A	O5X	90.76(18)	C6B	C7B	C2B	120.5(5)	C7D	C6D	C5D	118.8(5)
O1Y	Ca1B	O6Y	85.9(3)	O3C	B1CD	O2C	112.5(4)	C6D	C7D	C2D	120.8(5)
O2Y	Ca1B	O1Y	172.7(4)	O3C	B1CD	O2D	108.0(4)				
O2Y	Ca1B	O6Y	86.8(3)	O2D	B1CD	O2C	105.5(4)				
O3Y	Ca1B	O1Y	88.8(4)	O3D	B1CD	O2C	107.4(4)				
O3Y	Ca1B	O2Y	91.5(4)	O3D	B1CD	O3C	109.8(4)				
O3Y	Ca1B	O5Y	173.2(5)	O3D	B1CD	O2D	113.6(4)				
O3Y	Ca1B	O6Y	84.4(3)	C1C	O2C	B1CD	126.1(3)				
O4Y	Ca1B	O1Y	93.4(4)	C3C	O3C	B1CD	122.6(3)				
O4Y	Ca1B	O2Y	93.9(4)	O1C	C1C	O2C	119.4(4)				
O4Y	Ca1B	O3Y	95.3(4)	O1C	C1C	C2C	123.6(4)				
O4Y	Ca1B	O5Y	91.5(4)	O2C	C1C	C2C	117.0(4)				
O4Y	Ca1B	O6Y	179.2(5)	C3C	C2C	C1C	119.7(4)				
O5Y	Ca1B	O1Y	90.7(4)	C3C	C2C	C7C	119.7(4)				
O5Y	Ca1B	O2Y	88.1(4)	C7C	C2C	C1C	120.6(4)				
O5Y	Ca1B	O6Y	88.8(3)	O3C	C3C	C2C	121.7(4)				
O2A	B1AB	O2B	105.0(4)	O3C	C3C	C4C	119.0(4)				
O3A	B1AB	O2A	113.2(4)	C2C	C3C	C4C	119.4(4)				
O3A	B1AB	O2B	107.2(4)	C5C	C4C	C3C	120.1(5)				
O3B	B1AB	O2A	108.5(4)	C4C	C5C	C6C	120.8(4)				
O3B	B1AB	O3A	109.9(4)	C7C	C6C	C5C	120.2(5)				
O3B	B1AB	O2B	113.0(4)	C6C	C7C	C2C	119.9(5)				
C1A	O2A	B1AB	125.9(4)	C1D	O2D	B1CD	125.5(3)				
C3A	O3A	B1AB	122.0(4)	C3D	O3D	B1CD	121.6(3)				
O1A	C1A	O2A	119.9(4)	O1D	C1D	O2D	119.5(4)				
O1A	C1A	C2A	123.7(4)	O1D	C1D	C2D	123.7(4)				
O2A	C1A	C2A	116.5(4)	O2D	C1D	C2D	116.8(3)				
C3A	C2A	C1A	119.9(4)	C3D	C2D	C1D	119.9(4)				

Table S3. Bond Angles for CuSB.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1A[1]	Cu1	O1A[2]	164.74(8)	O3B	C3B	C4B	119.67(18)
O1B[3]	Cu1	O1A[1]	90.81(5)	C4B	C3B	C2B	119.10(18)
O1B	Cu1	O1A[2]	90.81(5)	C6B	C7B	C2B	119.9(2)
O1B	Cu1	O1A[1]	91.16(5)	C3A	C2A	C1A	118.38(18)
O1B[3]	Cu1	O1A[2]	91.16(5)	C3A	C2A	C7A	120.9(2)
O1B[3]	Cu1	O1B	165.14(8)	C7A	C2A	C1A	120.7(2)
C1A	O2A	B1	121.80(15)	O3A	C3A	C2A	121.23(18)
C1A	O1A	Cu1[4]	116.19(12)	O3A	C3A	C4A	119.7(2)
C1B	O1B	Cu1	116.46(12)	C4A	C3A	C2A	119.0(2)
C1B	O2B	B1	122.05(15)	C5B	C4B	C3B	119.5(2)
C3B	O3B	B1	119.29(15)	C4B	C5B	C6B	121.58(19)
C3A	O3A	B1	119.39(17)	C7B	C6B	C5B	119.5(2)
C3B	C2B	C1B	118.62(16)	O2B	B1	O2A	104.71(16)
C7B	C2B	C1B	120.85(17)	O3B	B1	O2A	107.54(16)
C7B	C2B	C3B	120.41(17)	O3B	B1	O2B	112.30(16)
O2A	C1A	C2A	119.39(16)	O3A	B1	O2A	111.90(16)
O1A	C1A	O2A	118.61(16)	O3A	B1	O2B	107.65(17)
O1A	C1A	C2A	121.96(17)	O3A	B1	O3B	112.52(18)
O1B	C1B	O2B	119.20(16)	C6A	C7A	C2A	119.6(3)
O1B	C1B	C2B	121.67(16)	C5A	C4A	C3A	119.0(3)
O2B	C1B	C2B	119.12(16)	C4A	C5A	C6A	121.9(3)
O3B	C3B	C2B	121.20(16)	C7A	C6A	C5A	119.5(3)

[1]+X,-1+Y,+Z; [2]3/2-X,-1+Y,1/2-Z; [3]3/2-X,+Y,1/2-Z; [4]+X,1+Y,+Z

Table S4. Bond Angles for LiSB.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1B	O2B	B1	121.6(6)	C5B	C6B	C7B	120.5(8)
C3B	O3B	B1	115.1(5)	C6B	C5B	C4B	120.7(8)
C1A	O2A	B1	122.2(5)	C7A	C2A	C1A	121.3(7)
C3A	O3A	B1	117.5(5)	C7A	C2A	C3A	118.7(6)
C1A	O1A	Li1[1]	127.2(6)	C3A	C2A	C1A	119.7(7)
Li1	O1W	Li1[2]	88.8(5)	O3A	C3A	C4A	117.9(6)
C1B	O1B	Li1	150.9(6)	O3A	C3A	C2A	121.6(6)
O3B	C3B	C2B	120.2(7)	C2A	C3A	C4A	120.5(7)
O3B	C3B	C4B	119.2(7)	O2B	B1	O2A	107.5(5)
C4B	C3B	C2B	120.6(6)	O3B	B1	O2B	112.8(5)
C3B	C2B	C1B	120.0(6)	O3B	B1	O2A	106.2(5)
C7B	C2B	C3B	119.0(7)	O3B	B1	O3A	109.0(6)
C7B	C2B	C1B	120.9(7)	O3A	B1	O2B	109.0(6)
O2A	C1A	C2A	117.3(7)	O3A	B1	O2A	112.4(5)
O1A	C1A	O2A	118.5(6)	O1A[3]	Li1	O1W	114.9(6)
O1A	C1A	C2A	124.1(7)	O1A[3]	Li1	O1W[2]	111.4(6)
O2B	C1B	C2B	116.5(6)	O1A[3]	Li1	Li1[2]	124.1(8)
O1B	C1B	O2B	119.9(7)	O1W	Li1	O1W[2]	91.2(5)
O1B	C1B	C2B	123.7(7)	O1W[2]	Li1	Li1[2]	43.9(4)
C5A	C4A	C3A	119.5(7)	O1W	Li1	Li1[2]	47.3(4)
C6A	C5A	C4A	120.5(7)	O1B	Li1	O1A[3]	128.7(6)
C2A	C7A	C6A	121.1(6)	O1B	Li1	O1W	99.1(6)
C3B	C4B	C5B	119.6(7)	O1B	Li1	O1W[2]	104.6(6)
C5A	C6A	C7A	119.7(7)	O1B	Li1	Li1[2]	107.1(7)
C2B	C7B	C6B	119.6(8)				

[1]+X,-1+Y,+Z; [2]1-X,2-Y,1-Z; [3]+X,1+Y,+Z

Section S2

Details on the calculation for spherical symmetry

At a point r from the center of a sphere with mass density ρ and stopping power S (with dimensions E/L) the flux of particles emitted by the element of volume dV at a distance r' from the point at r is

$$\mathrm{d}\varphi_E = \frac{s\mathrm{d}V}{4\pi r'^2} \qquad (S1)$$

The distance is given by $r'^2 = r^2 + R^2 - 2Rr\,cos\theta$. If r′ < range, the flux of particles at r is

$$\varphi(r) = \int_0^{2\pi} \mathrm{d}\eta \int_0^{\pi} \int_0^{R_{tot}} \frac{sR^2 sin\theta}{4\pi r'^2} \mathrm{d}\theta \mathrm{d}R = \frac{s}{2} \int_0^{\pi} \int_0^{R_{tot}} \frac{R^2}{r'^2} sin\theta \mathrm{d}\theta \mathrm{d}R \qquad (S2)$$

otherwise $\varphi(r) = 0$. The loss of energy occurs at the rate

$$\dot{D}(r) = \varphi \frac{S}{\rho} \qquad (S3)$$

That is

$$\dot{D}(r) = \frac{s}{2\rho} \int_0^{\pi} \int_0^{R_{tot}} S \frac{R^2}{r'^2} sin\theta \mathrm{d}\theta \mathrm{d}R \qquad (S4)$$

where S is a function of r', and having performed the integration on the azimuthal angle. The source term s is

$$s = \varphi_n \sigma \hat{\rho} \qquad (L^{-3}t^{-1}) \qquad (S5)$$

with φ_n being the neutron flux, σ the neutron capture cross section, and $\hat{\rho}$ the number density of the neutron absorbing nuclide. In the variables $x = r/R_{tot}$, $x' = r'/R_{tot}$, and $X = R/R_{tot}$ we have

$$\dot{D}(x) = \frac{1}{2} R_{tot} \varphi_n \sigma \frac{\hat{\rho}}{\rho} S \int_0^{\pi} \int_0^{1} \frac{X^2}{x'^2} sin\theta \mathrm{d}\theta \mathrm{d}X$$