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Crystal Structure of 2-[2-(4-Methylphenyl)Ethenyl]-1,3-Benzothiazole

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ABSTRACT

Single crystal x-ray diffraction analysis reveals that the compound 2-[2-(4-Methylphenyl)ethenyl]-1,3-benzothiazole crystallizes in Orthorhombic system with space group $Pc2_1b$ and the calculated lattice parameters are a=7.5371(2)Å, b=10.4767(3)Å, c=33.0684(5)Å, α=90°, β=90° and γ=90°. In the title compound the asymmetric unit contains two molecules. The dihedral angle between the benzothiazole ring and toluene ring is 9.3(3)° and 8.3(3)° in molecule A and B, respectively. The crystal packing is stabilized by intramolecular C-H…S type of hydrogen bond. In the crystal the two molecules are held together by C-H...π interactions in addition to Van Der Waals forces.

Keywords: Benzothiazole, Heterocyclic compounds, Sulfur atoms

INTRODUCTION

Benzothiazole belongs to the family of bicyclic heterocyclic compounds having benzene nucleus fused with five-membered ring comprising nitrogen and sulfur atoms. Benzothiazole is an important scaffold with a wide array of interesting biological activities and therapeutic applications. Benzothiazole derivatives have emerged as significant components in various therapeutic applications. The literature review reveals that benzothiazoles and their derivatives show considerable activity such as antitubercular [1], antimicrobial [2-5], anti-inflammatory [6], antitumor [7,8], anticonvulsant [9], antimalarial [10], anticancer [11], antidiabetic [12], antileishmanial [13], analgesic activity [14]. Benzothiazolesulfonamide provides inhibitors of HIV-1 protease with improved potency and antiviral activities [15]. Benzothiazole moiety has wide applications in dyes such as thioflavin [16]. In view of the importance of Benzothiazole derivatives, in the present communication we have report the synthesis and crystal structure of 2-[2-(4-Methylphenyl)ethenyl]-1,3-benzothiazole [17].

MATERIALS AND METHODS

4-Methylcinnamic acid (1 g, 6.16 mmol) and 2-aminothiophenol (0.64 mL, 6.28 mmol) were suspended in phosphorus oxychloride (10 ml) and then the reaction mixture was heated at 100°C under nitrogen atmosphere for 5 h. After the mixture had cooled to room temperature, it was carefully and slowly poured into a beaker of stirring distilled water (200 ml). The pH was adjusted to 7.0 by addition of sodium hydroxide pellets. The crude product was extracted with chloroform and washed with distilled water (200 ml) and brine (50 ml), dried over Na_2SO_4 and then solvent was removed using a rotary evaporator. The solvent was evaporated under reduced pressure to afford the crude product, which was purified by column chromatography (SiO_2), using n-Hexane-$CHCl_3$ (3:2) as eluent to give 2-[2-(4-Methylphenyl)ethenyl]-1,3-benzothiazole as colorless solid (1.45 g, 83%). M.P: 126-130°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.38 (s, 3H); 7.21 (d, *J*=7.8 Hz, 2H); 7.35 (t, *J*=8.1 Hz, 2H); 7.43-7.52 (m, 4H); 7.84 (d, *J*=7.8 Hz, 1H); 7.98 (d, *J*=8.1 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δc 21.4, 121.2, 121.4, 123.0, 125.2, 126.2, 127.4, 130.0, 133.0, 134.3, 138.0, 140.0, 154.0, 167.2.

RESULTS AND DISCUSSION

Crystal structure analysis

X-ray diffraction intensity data were collected at room temperature (293 K) on a Bruker axs SMART APEXII single crystal X-ray diffractometer equipped with graphite monochromatic Mo*Kα* (λ=0.71073 Å) radiation and CCD detector. The unit cell parameters were determined from 36 frames measured (0.5° phi-scan) from three different crystallographic zones using the method of difference vectors. The intensity data were collected with an average four-fold redundancy per reflection and optimum resolution (0.75 Å). The intensity data collection, frames integration, Lorentz and polarization corrections and decay correction were carried out using *SAINT-NT* (version 7.06a) software [18].

An empirical absorption correction (multi-scan) was performed using the *SADABS* program [18]. A total of 13410 reflections were collected and among them 5881reflections were found to be unique. Crystal structures were solved by direct methods using SHELXS-97 [19].

The structures were then refined by full matrix least- squares method using SHELXL-97 [19]. The computer programme XCAD4 reduced the data and the space group was deduced to be $Pc2_1b$ with lattice parameter a=7.5371(2) Å, b=10.4767(3) Å, c=33.0684(5) Å, α=90°, β =90° and γ=90°.

The crystal data and structure refinement parameters are given in Table 1. The atomic coordinates and their isotropic displacement parameters for non-hydrogen atoms are given in Table 2. The anisotropic displacement parameters are listed in Table 3. Selected bond distances and bond angles are given in Tables 4 and 5. The torsion angles involving non-hydrogen atoms are listed in Table 6. The various hydrogen bond geometrical parameters are presented in Table 7 with symmetry codes. The chemical diagram of the title compound is shown in Figure 1. The molecular structure (ORTEP diagram) of the compound is shown in Figure 2. The C-H…π interactions are shown in Figures 3 and 4 respectively.

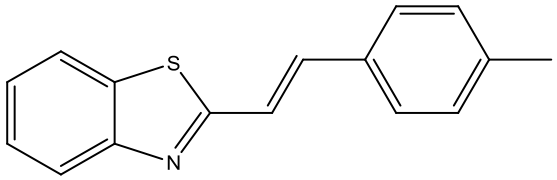

Figure 1: Schematic diagram of the title compound

Table 1: Crystal data and structure refinement of the title compound

Parameters	Values
Empirical formula	$C_{16}\,H_{13}\,N_1\,S_1$
Formula weight	251.33
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	"Orthorhombic", "P c 2_1 b"
Unit cell dimensions	a=7.5371(2) Å α=90°. b=10.4767(3) Å β=90°. c=33.0684(5) Å γ=90°.
Volume	2611.21(11) $Å^3$
Z, Calculated density	8, 1.279 Mg/m^3
Absorption coefficient	0.228 mm^{-1}
F(000)	1056
Crystal size	0.24 x 0.17 × 0.12 mm
Theta range for data collection	1.232 to 28.334 °.
Limiting indices	$-8 \le h \le 10$, $-13 \le k \le 13$, $-44 \le l \le 37$
Reflections collected/unique	13410/5881 [R(int)=0.0325]
Completeness to theta=25.242	99.60%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	5881/1/328
Goodness-of-fit on F^2	1.055
Final R indices [I>2 sigma(I)]	R1=0.0794, wR2=0.2251
R indices (all data)	R1=0.1165, wR2=0.2666
Extinction coefficient	0.0000(13)
Largest diff. peak and hole	0.730 and -0.353 $e.A^{-3}$

In the title compound, the asymmetric unit contains two molecules and there is a intramolecular C-H…S interaction which forms the S(5) ring motif which are shown in Figure 2. The benzothiazole ring is almost planar conformation with maximum deviation of atom C7 0.0426 (1) Å and C23 0.0655(1) Å in molecule A and B, respectively. The toluene ring is planar conformation with maximum deviation of atom C16 -0.0255(1) Å and C32 -0.0391 (1) Å in molecule A and B, respectively. The dihedral angle between the benzothiazole ring and toluene ring is 9.3(3)° and 8.3(3)° in molecule A and B, respectively. The carbon C8 & C9 atoms connected with the benzothiazole ring and toluene ring in molecule A and carbon C24 & C25 atoms in molecule B. It makes an extended conformation with the evidence from the torsion angle is [C7-C8-C9-C10]=-178.2° in molecule A and [C23-C24-C25-C26] =176.9° in molecule B.

The presence of double bond incorporated between the electron donor and electron acceptor can lead to trans to cis isomerization of twisted intramolecular charge transfer (TICT) state formation of benzothiazole moiety. The olefinic double bond is only trans, however gets converted to cis form for benzothiazole system in the presence of polar solvents [17].

Packing features

The crystal packing is stabilized by intramolecular C-H...S type of hydrogen bonds (C9-H9…S1 in molecule A and C25-H25…S2 in molecule B) which forms the S (5) ring motif which is shown in Figure 2 (Table 7). In the crystal, the two molecules are also held together by C-H…π interactions (Table 7), in addition to van der Waals forces. The C-H...π interaction is observed between the C5 atom and centroid of six member ring [C17-C18-C19-C20-C21-C22] with the distance of 3.613(1) Å and corresponding symmetry code is **Cg1**: -1+x, y, z shown in Figure 3.

The C-H...π interaction between the C16 atom and centroid of five member ring [C17-C22-N2-C23-S2] with the distance of 3.704(2) Å and corresponding symmetry code is **Cg2:** 1-x, ½+y, -z shown in Figure 3.

Another C-H…π interaction between the C18 atom and the centroid of six member ring [C1-C2-C3-C4-C5-C6] with the distance of 3.574(1) Å and corresponding symmetry code is **Cg3**: x, y, z shown in Figure 4.

Table 2: Atomic coordinates(x10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for the non-hydrogen atoms

Atom	X	Y	Z	*U(eq.)
C1	5164(9)	7810(1)	1717(2)	52(1)
C2	5800(1)	8438(1)	2074(2)	61(1)
C3	5428(1)	7853(2)	2435(3)	65(1)
C4	4532(1)	6709(3)	2453(3)	73(2)
C5	3877(1)	6130(1)	2113(2)	64(4)
C6	4176(9)	6712(9)	1746(2)	48(1)
C7	4630(1)	7536(8)	1055(2)	53(3)
C8	4770(8)	7765(6)	633(2)	44(1)
C9	4118(1)	7130(2)	354(2)	67(1)
C10	4174(8)	7217(8)	-81(2)	44(1)
C11	5159(1)	8127(1)	-275(2)	56(1)
C12	5332(2)	8179(9)	-698(3)	57(3)
C13	4380(1)	7289(1)	-935(2)	53(1)
C14	3388(1)	6386(1)	-742(3)	57(1)
C15	3273(9)	6348(1)	-323(3)	55(3)
C16	4560(1)	7336(3)	-1377(3)	86(1)
C17	9167(9)	4872(9)	1747(2)	48(1)
C18	8850(1)	5468(1)	2120(2)	57(1)
C19	9548(9)	4867(1)	2468(3)	63(1)
C20	10461(1)	3740(2)	2446(3)	71(2)
C21	10744(1)	3154(1)	2075(2)	63(1)
C22	10110(1)	3711(8)	1722(2)	42(2)
C23	9621(1)	4102(2)	1082(3)	74(2)
C24	9845(5)	3978(7)	634(3)	132(1)
C25	9021(1)	4601(9)	353(3)	56(1)
C26	9188(9)	4427(9)	-85(2)	48(1)
C27	10194(9)	3457(9)	-284(2)	49(1)
C28	10233(1)	3451(1)	-699(3)	54(1)
C29	9437(1)	4318(1)	-937(2)	48(3)
C30	8413(1)	5250(1)	-736(2)	55(2)
C31	8300(1)	5283(1)	-322(2)	54(3)
C32	9563(3)	4296(4)	-1395(2)	79(2)
S1	3538(3)	6236(2)	1276(7)	629(1)
S2	8534(3)	5348(2)	1276(7)	598(1)
N1	5356(8)	8358(6)	1306(7)	383(1)
N2	10372(9)	3244(6)	1302(6)	34(1)

*Ueq=(1/3)ΣiΣjUij ai*aj*ai.aj

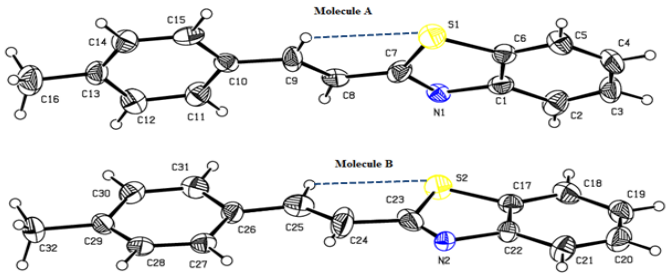

Figure 2: The molecular structure of the compound, showing the atom labeling and displacement ellipsoids drawn at the 30% probability level. The intramolecular C-H…S interaction is shown as a dashed line

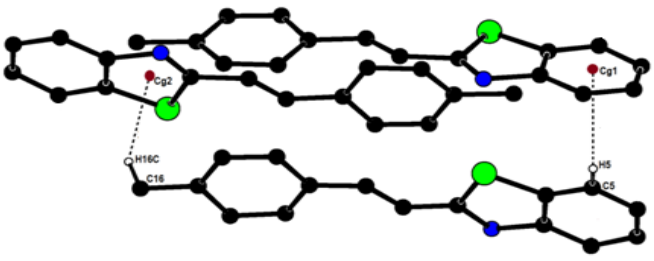

Figure 3: C—H...*π* interaction of the compound

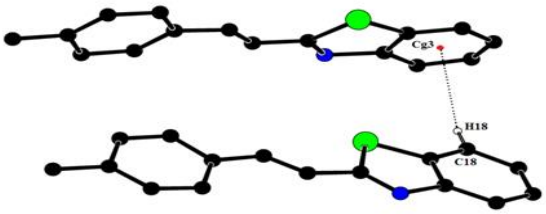

Figure 4: C—H...π interaction of the compound

Table 3: Anisotropic displacement parameters ($Å^2$ x10^3) for the non-hydrogen atoms

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	37(4)	60(5)	56(5)	8(4)	-2(3)	3(4)
C2	68(5)	55(6)	58(5)	-12(4)	-10(4)	1(5)
C3	74(6)	79(7)	39(4)	-14(5)	-1(5)	19(6)
C4	65(5)	106(9)	46(5)	-5(5)	19(5)	16(6)
C5	60(5)	77(8)	54(5)	11(6)	13(4)	-5(5)
C6	42(4)	52(5)	48(4)	-5(4)	0(3)	2(4)
C7	51(4)	56(5)	51(4)	-15(4)	-12(3)	-2(4)
C8	36(3)	33(3)	60(4)	4(3)	3(3)	-22(3)
C9	66(5)	104(8)	32(3)	3(4)	0(3)	51(5)
C10	37(4)	45(5)	51(4)	9(4)	4(3)	12(3)
C11	62(5)	51(5)	56(5)	-10(4)	-7(4)	-1(5)
C12	68(5)	45(4)	57(5)	5(4)	7(4)	5(4)
C13	58(5)	61(6)	41(4)	-8(4)	-4(4)	15(5)
C14	56(5)	55(6)	59(5)	-12(5)	-2(4)	-8(4)
C15	36(3)	49(5)	81(6)	-2(6)	-7(4)	-9(4)
C16	96(8)	103(2)	55(5)	-18(7)	-4(5)	31(8)
C17	40(4)	49(5)	52(5)	-8(4)	4(3)	-5(4)
C18	52(4)	54(6)	64(6)	-8(5)	12(4)	0(4)
C19	60(5)	75(7)	51(5)	-18(5)	8(5)	-17(5)
C20	68(6)	86(8)	55(5)	18(6)	-10(5)	-13(6)
C21	72(5)	59(6)	55(5)	4(5)	-14(4)	6(5)
C22	48(4)	39(4)	40(4)	2(3)	-2(3)	1(4)
C23	54(5)	113(9)	55(5)	-30(6)	16(4)	-48(5)
C24	106(8)	246(8)	44(5)	21(7)	-17(5)	-109(2)
C25	51(4)	39(4)	79(6)	6(4)	2(4)	16(3)
C26	50(4)	54(5)	40(4)	2(4)	-2(3)	-12(4)
C27	41(4)	49(5)	55(5)	2(4)	-2(3)	6(4)
C28	37(3)	66(6)	59(5)	-3(5)	2(3)	16(4)
C29	46(4)	57(5)	42(4)	-8(4)	7(3)	-10(4)
C30	52(4)	53(5)	57(5)	5(5)	-9(4)	-5(4)
C31	52(4)	47(5)	62(5)	-16(5)	5(4)	-5(4)
C32	72(6)	125(2)	40(4)	-7(6)	6(4)	-11(7)
S1	65(1)	63(1)	62(1)	-6(1)	0(1)	-13(3)
S2	64(4)	53(4)	62(5)	1(3)	0(1)	9(2)
N1	37(3)	33(3)	45(3)	-2(3)	5(2)	-13(3)
N2	39(3)	27(3)	36(3)	5(3)	-3(2)	8(2)

The anisotropic displacement factor takes the form: $\exp\{-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hk\, a^* b^* U_{12}]\}$

Table 4: Selected Bond lengths [Å] of the title compound

Bond	Bond length [Å]
C(1)-C(6)	1.374(12)
C(1)-C(2)	1.434(11)
C(1)-N(1)	1.481(10)
C(2)-C(3)	1.371(13)
C(3)-C(4)	1.377(15)
C(4)-C(5)	1.370(14)
C(5)-C(6)	1.376(11)
C(6)-S(1)	1.699(8)
C(7)-N(1)	1.316(9)
C(7)-C(8)	1.422(11)
C(7)-S(1)	1.751(9)
C(8)-C(9)	1.238(12)
C(9)-C(10)	1.442(10)
C(10)-C(11)	1.368(12)
C(10)-C(15)	1.390(12)
C(11)-C(12)	1.405(12)
C(12)-C(13)	1.414(13)
C(13)-C(14)	1.364(13)
C(13)-C(16)	1.471(12)
C(14)-C(15)	1.389(10)
C(17)-C(18)	1.403(11)
C(17)-C(22)	1.410(11)
C(17)-S(2)	1.703(8)
C(18)-C(19)	1.414(14)
C(19)-C(20)	1.369(14)
C(20)-C(21)	1.388(14)
C(21)-C(22)	1.390(10)
C(22)-N(2)	1.486(9)
C(23)-N(2)	1.288(13)
C(23)-C(24)	1.487(13)
C(23)-S(2)	1.670(12)
C(24)-C(25)	1.228(15)
C(25)-C(26)	1.465(12)
C(26)-C(31)	1.366(13)
C(26)-C(27)	1.429(12)
C(27)-C(28)	1.373(11)
C(28)-C(29)	1.344(12)
C(29)-C(30)	1.412(13)
C(29)-C(32)	1.520(10)
C(30)-C(31)	1.371(10)

Computational details

Data collection: SMART [18], cell refinement: SAINT [18], data reduction: SAINT; program(s) used to solve structure: SHELXS97 [19], program(s) used to refine structure: SHELXL97 [19], Images were created with the ORTEP-PLATON program [20,21], software used to prepare material for publication: SHELXL97 and PARST [22].

Table 5: Selected bond angles [°] of the title compound

Bond	Bond Angle [°]
C(6)-C(1)-C(2)	120.5(8)
C(6)-C(1)-N(1)	116.2(8)
C(2)-C(1)-N(1)	122.9(8)
C(3)-C(2)-C(1)	116.3(9)
C(2)-C(3)-C(4)	121.8(10)
C(5)-C(4)-C(3)	121.8(11)
C(4)-C(5)-C(6)	117.9(11)
C(1)-C(6)-C(5)	121.5(9)
C(1)-C(6)-S(1)	109.6(7)
C(5)-C(6)-S(1)	128.9(8)
N(1)-C(7)-C(8)	118.6(7)
N(1)-C(7)-S(1)	116.2(6)
C(8)-C(7)-S(1)	125.3(5)
C(9)-C(8)-C(7)	127.6(7)
C(8)-C(9)-C(10)	134.1(11)
C(11)-C(10)-C(15)	116.9(8)
C(11)-C(10)-C(9)	121.9(9)
C(15)-C(10)-C(9)	121.3(9)
C(10)-C(11)-C(12)	122.9(8)
C(11)-C(12)-C(13)	118.6(8)
C(14)-C(13)-C(12)	118.4(7)
C(14)-C(13)-C(16)	122.6(9)
C(12)-C(13)-C(16)	118.9(9)
C(13)-C(14)-C(15)	121.4(8)
C(10)-C(15)-C(14)	121.7(8)
C(18)-C(17)-C(22)	121.4(8)
C(18)-C(17)-S(2)	128.7(7)
C(22)-C(17)-S(2)	109.9(6)
C(17)-C(18)-C(19)	117.1(9)
C(20)-C(19)-C(18)	121.8(10)
C(19)-C(20)-C(21)	120.4(10)
C(20)-C(21)-C(22)	120.2(9)
C(21)-C(22)-C(17)	119.1(8)
C(21)-C(22)-N(2)	126.9(7)
C(17)-C(22)-N(2)	113.9(7)
N(2)-C(23)-C(24)	119.8(11)
N(2)-C(23)-S(2)	122.9(6)
C(24)-C(23)-S(2)	117.3(11)
C(25)-C(24)-C(23)	134.6(16)
C(24)-C(25)-C(26)	130.4(11)
C(31)-C(26)-C(27)	117.6(7)
C(31)-C(26)-C(25)	116.3(8)
C(27)-C(26)-C(25)	126.1(8)
C(28)-C(27)-C(26)	118.3(8)

C(29)-C(28)-C(27)	125.0(8)
C(28)-C(29)-C(30)	115.8(7)
C(28)-C(29)-C(32)	123.1(9)
C(30)-C(29)-C(32)	121.0(9)
C(31)-C(30)-C(29)	121.4(9)
C(26)-C(31)-C(30)	121.7(9)
C(7)-N(1)-C(1)	106.5(7)
C(23)-N(2)-C(22)	103.9(7)
C(6)-S(1)-C(7)	91.2(4)
C(23)-S(2)-C(17)	89.2(5)

Table 6: Selected Torsion angle of the title compound

	Torsion angle [°]
N(1)-C(1)-C(2)-C(3)	176.0(8)
N(1)-C(1)-C(6)-C(5)	-178.7(8)
C(2)-C(1)-C(6)-S(1)	177.3(7)
C(4)-C(5)-C(6)-S(1)	-179.9(7)
N(1)-C(7)-C(8)-C(9)	-177.0(8)
C(7)-C(8)-C(9)-C(10)	-178.2(8)
C(8)-C(9)-C(10)-C(15)	-179.5(9)
C(9)-C(10)-C(11)-C(12)	175.6(8)
C(11)-C(12)-C(13)-C(16)	-179.8(9)
C(16)-C(13)-C(14)-C(15)	178.6(9)
C(9)-C(10)-C(15)-C(14)	-176.8(8)
S(2)-C(17)-C(18)-C(19)	-179.4(6)
C(20)-C(21)-C(22)-N(2)	176.9(8)
S(2)-C(17)-C(22)-C(21)	-179.8(7)
C(18)-C(17)-C(22)-N(2)	-178.0(7)
N(2)-C(23)-C(24)-C(25)	177.6(11)
C(23)-C(24)-C(25)-C(26)	176.9(9)
C(24)-C(25)-C(26)-C(31)	179.0(10)
C(25)-C(26)-C(27)-C(28)	-178.7(8)
C(27)-C(28)-C(29)-C(32)	178.1(8)
C(32)-C(29)-C(30)-C(31)	-179.6(9)
C(25)-C(26)-C(31)-C(30)	177.3(8)
C(8)-C(7)-N(1)-C(1)	-174.3(7)
C(2)-C(1)-N(1)-C(7)	-179.9(8)
C(24)-C(23)-N(2)-C(22)	178.7(7)
C(21)-C(22)-N(2)-C(23)	-177.0(8)
C(5)-C(6)-S(1)-C(7)	-177.5(9)
C(8)-C(7)-S(1)-C(6)	176.5(7)
C(24)-C(23)-S(2)-C(17)	-177.7(6)
C(18)-C(17)-S(2)-C(23)	177.0(8)

Table 7: Hydrogen bonds ofthe title compound

D—H…A	D—H(Å)	H…A(Å)	D…A(Å)	D—H…A[°]
C9-H9…S1[i]	0.93	2.76	3.222(8)	112
C25-H25…S2 [i]	0.93	2.80	3.174(10)	105
C5-H5...Cg1 [ii]	0.93	2.68	3.691(2)	149
C16-H16C...Cg2 [iii]	0.93	2.77	3.704(3)	153
C18-H18...Cg3 [i]	0.93	2.64	3.574(1)	144

Symmetry codes: i) x, y, z; ii) -1+x, y, z; iii) 1-x, ½+y, -z

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