## **Supporting Information**

## Structural diversity and photocatalytic activities of six Co(II)/Ni(II) complexes with three flexible phenylenediacetate isomers

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Fig. S1 View of the 1D loop containing polymer chain of 1 along *ab* plan.



Fig. S2 Ball-and-stick view of 2D layer along *ac* plan in 4.



Fig. S3 Ball-and-stick view of 2D layer along *ab* plan in 6.



(1)



(2)



(3)



(4)



(5)



**Fig. S4** Coordination modes and conformations of bis(1-imidazoly)benzene (bib) ligands in complexes **1-6**.







Fig. S6 Thermal gravimetric analysis (TGA) curves of complexes 1-6.



Fig. S7 The PXRD pattern of the complex 4 before and after photocatalytic reaction.



Fig. S8 Photocatalytic degradation of MB as a function of irradiation time for different samples without  $H_2O_2$ .



Fig. S9 Photodegradation efficiency of MB in the presence of TBA scavenger over complex 4.









(c)

Fig. S10 Cyclic voltammograms of complexes 4–6 (a for 4, b for 5, c for 6).



**Fig. S11** Electrochemical impedance spectroscopy (EIS) Nyquist plots of complexes 1–3 and blank nickel foam tested in 0.1 M KOH.

BondDist.BondDist.BondDist.N(1)-O(1)2.068(2)Ni(2)-O(3)2.055(2)Ni(1)-N(H2)2.069(2)N(1)-O(3)2.068(2)Ni(2)-O(6)2.128(2)Ni(2)-N(5)2.097(3)N(1)-O(3)2.099(2)Ni(2)-O(6)2.128(2)Ni(2)-N(5)2.097(3)N(1)-O(3)2.099(2)Ni(2)-N(1)2.069(2)Ni(2)-N(5)2.081(2)Angle(*)Angle(*)Angle(*)O(1A)-Ni(1)-O(1)18.0N(4C)-Ni(1)-O(8)87.56'9)O(4)-Ni(2)-O(6)9.99(9)O(1A)-Ni(1)-O(3)88.09(9)N(4C)-Ni(1)-O(8)87.56'9)O(4)-Ni(2)-N(5)88.71(9)O(1A)-Ni(1)-O(8A)91.91(9)N(4B)-Ni(1)-O(8)87.56'9)O(4)-Ni(2)-N(5)88.71(9)O(1A)-Ni(1)-O(8A)91.91(9)N(4D)-Ni(1)-N(4B)180.0N(1)-Ni(2)-O(6)89.48(10)O(1A)-Ni(1)-N(4C)88.67(9)O(3)-Ni(2)-O(1)174.62(8)N(1)-Ni(2)-N(5)91.71(9)O(1A)-Ni(1)-N(4B)91.36(9)O(3)-Ni(2)-N(1)88.72(9)N(5)-Ni(2)-N(6)86.64(11)O(1)-Ni(1)-N(4B)91.36(9)O(3)-Ni(2)-N(5)91.57(10)N(5)-Ni(2)-N(6)86.64(11)O(1)-Ni(1)-N(4B)91.36(9)O(3)-Ni(2)-N(5)91.57(10)N(5)-Ni(2)-N(6)86.64(11)O(1)-Ni(1)-N(4B)91.36(9)O(3)-Ni(2)-N(5)91.57(10)N(5)-Ni(2)-N(6)86.64(11)O(1)-Ni(1)-N(4B)91.36(9)O(3)-Ni(2)-N(5)91.57(10)N(5)-Ni(2)-O(6)174.66(9)O(1)-Ni(1)-N(4B)91.36(9)O(3	1						
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O(1A)-Ni(1)-N(4C)88.67(9) $O(3)-Ni(2)-O(4)$ 174.62(8) $N(1)-Ni(2)-N(5)$ 176.11(10) $O(1)-Ni(1)-N(4C)$ 91.33(9) $O(3)-Ni(2)-O(6)$ 90.14(9) $N(1)-Ni(2)-N(8D)$ 94.17(9) $O(1)-Ni(1)-N(4B)$ 88.67(9) $O(3)-Ni(2)-N(1)$ 88.72(9) $N(5)-Ni(2)-O(6)$ 86.64(11) $O(1A)-Ni(1)-N(4B)$ 91.33(9) $O(3)-Ni(2)-N(5)$ 91.57(10) $N(5)-Ni(2)-N(8D)$ 89.72(10) $O(8)-Ni(1)-O(8A)$ 180.0 $O(3)-Ni(2)-N(8D)$ 86.06(9) $N(8D)-Ni(2)-O(6)$ 174.66(9) $O(8)-Ni(1)-O(1A)$ 2.1186(16) $Ni(1)-O(2A)$ 2.136(2) $Ni(1)-O(3)$ 2.116(2) $Ni(1)-O(1A)$ 2.1186(16) $Ni(1)-O(2A)$ 2.136(2) $Ni(1)-O(4)$ 2.025(3) $Angle$ (°) $Angle$ (°) $Angle$ (°) $O(1A)-Ni(1)-O(2A)$ 91.97(10) $O(2A)-Ni(1)-O(4)$ 105.46(8) $O(3)-Ni(1)-O(1A)$ 105.01(8) $O(3)-Ni(1)-O(2A)$ 91.97(10) $O(3)-Ni(1)-O(4)$ 156.37(8) $N(1)-Ni(1)-O(1A)$ 97.32(8) $N(1A)-Ni(1)-O(1A)$ 95.27(8) $N(4A)-Ni(1)-N(1)$ 2.80(10) $N(4A)-Ni(1)-O(3)$ 89.43(10) $N(4A)-Ni(1)-O(1A)$ 95.98(9) $N(4A)-Ni(1)-N(1)$ 2.80(10) $N(1)-O(1)$ 2.154(2	O(1A)-Ni(1)-O(8)	88.09(9)	N(4C)-Ni(1)-N(4B)	180.0	N(1)-Ni(2)-O(6)	89.48(10)	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(1A)-Ni(1)-N(4C)	88.67(9)	O(3)-Ni(2)-O(4)	174.62(8)	N(1)-Ni(2)-N(5)	176.11(10)	
O(1)-Ni(1)-N(4B)88.67(9) $O(3)$ -Ni(2)-N(1)88.72(9)N(5)-Ni(2)-O(6)86.64(11) $O(1A)$ -Ni(1)-O(4B)91.33(9) $O(3)$ -Ni(2)-N(5)91.57(10)N(5)-Ni(2)-N(8D)89.72(10) $O(8)$ -Ni(1)-O(8A)180.0 $O(3)$ -Ni(2)-N(8D)86.06(9)N(8D)-Ni(2)-O(6)174.66(9)ZBondDist.BondDist.BondDist.BondDist.N(1)-O(1A)2.1186(16)Ni(1)-O(2A)2.136(2)Ni(1)-O(3)2.116(2)Ni(1)-O(4)2.1366(18)Ni(1)-N(1)2.041(2)Ni(1)-N(4A)2.025(3)Angle(°)Angle(°)Angle(°)O(1A)-Ni(1)-O(2A)61.61(7)O(1A)-Ni(1)-O(4)162.55(8)O(2A)-Ni(1)-O(4)105.46(8)O(3)-Ni(1)-O(1A)105.01(8)O(3)-Ni(1)-O(2A)91.97(10)O(3)-Ni(1)-O(4)157.26(8)N(1)-Ni(1)-O(1A)97.32(8)N(1A)-Ni(1)-O(1A)95.27(8)N(4A)-Ni(1)-O(2A)156.37(8)N(4A)-Ni(1)-O(3)89.43(10)N(4A)-Ni(1)-O(4)95.98(9)N(4A)-Ni(1)-O(2A)156.37(8)BondDist.BondDist.BondDist.BondDist.Ni(1)-O(1)2.154(2)Ni(1)-O(2)2.091(2)Ni(1)-O(3A)2.083(2)Ni(1)-O(4A)2.153(2)Ni(1)-N(1)2.023(2)Ni(1)-N(4B)2.039(2)	O(1)-Ni(1)-N(4C)	91.33(9)	O(3)-Ni(2)-O(6)	90.14(9)	N(1)-Ni(2)-N(8D)	94.17(9)	
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O(8)-Ni(1)-O(8A)         180.0         O(3)-Ni(2)-N(8D)         86.06(9)         N(8D)-Ni(2)-O(6)         174.66(9)           Z         Z           Bond         Dist.         Bond         Dist.         Bond         Dist.           Ni(1)-O(1A)         2.1186(16)         Ni(1)-O(2A)         2.136(2)         Ni(1)-O(3)         2.116(2)           Ni(1)-O(4)         2.1366(18)         Ni(1)-N(1)         2.041(2)         Ni(1)-N(4A)         2.025(3)           Angle         (°)         Angle         (°)         Angle         (°)         Angle         (°)           O(1A)-Ni(1)-O(4)         165.01(8)         O(3)-Ni(1)-O(4)         162.55(8)         O(2A)-Ni(1)-O(4)         105.46(8)           O(3)-Ni(1)-O(1A)         105.01(8)         O(3)-Ni(1)-O(2A)         91.97(10)         O(3)-Ni(1)-O(4)         61.86(7)           N(1)-Ni(1)-O(1A)         97.32(8)         N(1A)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-O(2A)         156.37(8)           N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(4)         95.98(9)         N(4A)-Ni(1)-N(1)         92.80(10)           Bond         Dist.         Bond         Dist.         Bond         Dist.           Bond         Dist.         Bond         Dist.         Bon	O(1A)-Ni(1)-N(4B)	91.33(9)	O(3)-Ni(2)-N(5)	91.57(10)	N(5)-Ni(2)-N(8D)	89.72(10)	
Bond         Dist.         Bond         Dist.         Bond         Dist.           Ni(1)-O(1A)         2.1186(16)         Ni(1)-O(2A)         2.136(2)         Ni(1)-O(3)         2.116(2)           Ni(1)-O(4)         2.1366(18)         Ni(1)-N(1)         2.041(2)         Ni(1)-N(4A)         2.025(3)           Angle         (°)         Angle         (°)         Angle         (°)           O(1A)-Ni(1)-O(2A)         61.61(7)         O(1A)-Ni(1)-O(4)         162.55(8)         O(2A)-Ni(1)-O(4)         105.46(8)           O(3)-Ni(1)-O(1A)         105.01(8)         O(3)-Ni(1)-O(2A)         91.97(10)         O(3)-Ni(1)-O(4)         157.26(8)           N(1)-Ni(1)-O(1A)         97.32(8)         N(1)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-O(2A)         156.37(8)           N(4A)-Ni(1)-O(4)         95.41(8)         N(4A)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-O(2A)         156.37(8)           N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-N(1)         92.80(10)           N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(1A)         95.98(9)         N(4A)-Ni(1)-N(1)         92.80(10)           Ni(1)-O(1)         2.154(2)         Ni(1)-O(2)         2.091(2)         Ni(1)-O(3A)         2.	O(8)-Ni(1)-O(8A)	180.0	O(3)-Ni(2)-N(8D)	86.06(9)	N(8D)-Ni(2)-O(6)	174.66(9)	
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Ni(1)-O(4)         2.1366(18)         Ni(1)-N(1)         2.041(2)         Ni(1)-N(4A)         2.025(3)           Angle         (°)         Angle         (°)         Angle         (°)         Angle         (°)           O(1A)-Ni(1)-O(2A)         61.61(7)         O(1A)-Ni(1)-O(4)         162.55(8)         O(2A)-Ni(1)-O(4)         105.46(8)           O(3)-Ni(1)-O(1A)         105.01(8)         O(3)-Ni(1)-O(2A)         91.97(10)         O(3)-Ni(1)-O(4)         61.86(7)           N(1)-Ni(1)-O(1A)         97.32(8)         N(1)-Ni(1)-O(2A)         94.92(10)         N(1)-Ni(1)-O(3)         157.26(8)           N(1)-Ni(1)-O(4)         95.41(8)         N(4A)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-O(2A)         156.37(8)           N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(4)         95.98(9)         N(4A)-Ni(1)-N(1)         92.80(10)           J           J           J           J           J           J           J           J           J           J           J           J            J	Ni(1)-O(1A)	2.1186(16)	Ni(1)-O(2A)	2.136(2)	Ni(1)-O(3)	2.116(2)	
Angle(°)Angle(°)Angle(°)O(1A)-Ni(1)-O(2A)61.61(7)O(1A)-Ni(1)-O(4)162.55(8)O(2A)-Ni(1)-O(4)105.46(8)O(3)-Ni(1)-O(1A)105.01(8)O(3)-Ni(1)-O(2A)91.97(10)O(3)-Ni(1)-O(4)61.86(7)N(1)-Ni(1)-O(1A)97.32(8)N(1)-Ni(1)-O(2A)94.92(10)N(1)-Ni(1)-O(3)157.26(8)N(1)-Ni(1)-O(4)95.41(8)N(4A)-Ni(1)-O(1A)95.27(8)N(4A)-Ni(1)-O(2A)156.37(8)N(4A)-Ni(1)-O(3)89.43(10)N(4A)-Ni(1)-O(4)95.98(9)N(4A)-Ni(1)-N(1)92.80(10)JBondDist.BondDist.Ni(1)-O(1)2.154(2)Ni(1)-O(2)2.091(2)Ni(1)-O(3A)2.083(2)Ni(1)-O(4A)2.153(2)Ni(1)-N(1)2.023(2)Ni(1)-N(4B)2.039(2)	Ni(1)-O(4)	2.1366(18)	Ni(1)-N(1)	2.041(2)	Ni(1)-N(4A)	2.025(3)	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Angle	(°)	Angle	(°)	Angle	(°)	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(1A)-Ni(1)-O(2A)	61.61(7)	O(1A)-Ni(1)-O(4)	162.55(8)	O(2A)-Ni(1)-O(4)	105.46(8)	
N(1)-Ni(1)-O(1A)       97.32(8)       N(1)-Ni(1)-O(2A)       94.92(10)       N(1)-Ni(1)-O(3)       157.26(8)         N(1)-Ni(1)-O(4)       95.41(8)       N(4A)-Ni(1)-O(1A)       95.27(8)       N(4A)-Ni(1)-O(2A)       156.37(8)         N(4A)-Ni(1)-O(3)       89.43(10)       N(4A)-Ni(1)-O(4)       95.98(9)       N(4A)-Ni(1)-N(1)       92.80(10)         J         Bond       Dist.       Bond       Dist.         Ni(1)-O(1)       2.154(2)       Ni(1)-O(2)       2.091(2)       Ni(1)-O(3A)       2.083(2)         Ni(1)-O(4A)       2.153(2)       Ni(1)-N(1)       2.023(2)       Ni(1)-N(4B)       2.039(2)	O(3)-Ni(1)-O(1A)	105.01(8)	O(3)-Ni(1)-O(2A)	91.97(10)	O(3)-Ni(1)-O(4)	61.86(7)	
N(1)-Ni(1)-O(4)         95.41(8)         N(4A)-Ni(1)-O(1A)         95.27(8)         N(4A)-Ni(1)-O(2A)         156.37(8)           N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(4)         95.98(9)         N(4A)-Ni(1)-N(1)         92.80(10)           J           Bond         Dist.         Bond         Dist.           Ni(1)-O(1)         2.154(2)         Ni(1)-O(2)         2.091(2)         Ni(1)-O(3A)         2.083(2)           Ni(1)-O(4A)         2.153(2)         Ni(1)-N(1)         2.023(2)         Ni(1)-N(4B)         2.039(2)	N(1)-Ni(1)-O(1A)	97.32(8)	N(1)-Ni(1)-O(2A)	94.92(10)	N(1)-Ni(1)-O(3)	157.26(8)	
N(4A)-Ni(1)-O(3)         89.43(10)         N(4A)-Ni(1)-O(4)         95.98(9)         N(4A)-Ni(1)-N(1)         92.80(10)           J <thj< th="">         J         <thj< th=""> <thj< td=""><td>N(1)-Ni(1)-O(4)</td><td>95.41(8)</td><td>N(4A)-Ni(1)-O(1A)</td><td>95.27(8)</td><td>N(4A)-Ni(1)-O(2A)</td><td>156.37(8)</td></thj<></thj<></thj<>	N(1)-Ni(1)-O(4)	95.41(8)	N(4A)-Ni(1)-O(1A)	95.27(8)	N(4A)-Ni(1)-O(2A)	156.37(8)	
Bond         Dist.         Bond         Dist.         Bond         Dist.           Ni(1)-O(1)         2.154(2)         Ni(1)-O(2)         2.091(2)         Ni(1)-O(3A)         2.083(2)           Ni(1)-O(4A)         2.153(2)         Ni(1)-N(1)         2.023(2)         Ni(1)-N(4B)         2.039(2)	N(4A)-Ni(1)-O(3)	89.43(10)	N(4A)-Ni(1)-O(4)	95.98(9)	N(4A)-Ni(1)-N(1)	92.80(10)	
Bond         Dist.         Bond         Dist.         Bond         Dist.           Ni(1)-O(1)         2.154(2)         Ni(1)-O(2)         2.091(2)         Ni(1)-O(3A)         2.083(2)           Ni(1)-O(4A)         2.153(2)         Ni(1)-N(1)         2.023(2)         Ni(1)-N(4B)         2.039(2)	3						
Ni(1)-O(1)2.154(2)Ni(1)-O(2)2.091(2)Ni(1)-O(3A)2.083(2)Ni(1)-O(4A)2.153(2)Ni(1)-N(1)2.023(2)Ni(1)-N(4B)2.039(2)	Bond	Dist.	Bond	Dist.	Bond	Dist.	
Ni(1)-O(4A) 2.153(2) Ni(1)-N(1) 2.023(2) Ni(1)-N(4B) 2.039(2)	Ni(1)-O(1)	2.154(2)	Ni(1)-O(2)	2.091(2)	Ni(1)-O(3A)	2.083(2)	
	Ni(1)-O(4A)	2.153(2)	Ni(1)-N(1)	2.023(2)	Ni(1)-N(4B)	2.039(2)	

 Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for Complexes 1-6.

Angle	(°)	Angle	(°)	Angle	(°)
O(2)-Ni(1)-O(1)	62.31(7)	O(2)-Ni(1)-O(4A)	100.32(9)	O(3A)-Ni(1)-O(1)	98.38(8)
O(3A)-Ni(1)-O(2)	155.68(8)	O(3A)-Ni(1)-O(4A)	62.21(8)	O(4A)-Ni(1)-O(1)	87.80(8)
N(1)-Ni(1)-O(1)	90.35(9)	N(1)-Ni(1)-O(2)	98.80(9)	N(1)-Ni(1)-O(3A)	95.77(9)
N(1)-Ni(1)-O(4A)	157.30(10)	N(1)-Ni(1)-N(4B)	96.97(10)	N(4B)-Ni(1)-O(1)	162.85(9)
N(4B)-Ni(1)-O(2)	101.12(8)	N(4B)-Ni(1)-O(3A)	96.29(9)	N(4B)-Ni(1)-O(4A)	91.23(9)

Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(4)	2.158(2)	Co(1)-O(2A)	1.996(2)	Co(1)-O(3)	2.273(3)
Co(1)-O(5)	2.149(3)	Co(1)-N(1)	2.118(3)	Co(1)-N(4B)	2.107(3)
Angle	(°)	Angle	(°)	Angle	(°)
O(1)-Co(1)-O(2)	59.63(9)	O(4A)-Co(1)-O(2)	160.99(11)	O(4A)-Co(1)-O(1)	101.37(10)
O(4A)-Co(1)-O(5)	93.95(12)	O(4A)-Co(1)-N(4B)	92.53(12)	O(4A)-Co(1)-N(1)	88.41(12)
O(5)-Co(1)-O(2)	104.93(11)	O(5)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(2)	88.88(11)
N(4B)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(5)	92.45(11)	N(4B)-Co(1)-N(1)	178.93(12)
N(1)-Co(1)-O(2)	90.39(11)	N(1)-Co(1)-O(1)	88.76(10)	N(1)-Co(1)-O(5)	86.98(11)

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Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(2)	2.206(3)	Co(1)-O(1)	2.199(2)	Co(1)-O(4A)	2.042(3)
Co(1)-O(3A)	2.149(3)	Co(1)-N(1)	2.064(2)	Co(1)-N(5)	2.043(2)
Angle	(°)	Angle	(°)	Angle	(°)
O(4)-Co(1)-O(3)	58.14(7)	O(2A)-Co(1)-O(4)	94.97(8)	O(2A)-Co(1)-O(3)	145.43(9)
O(2A)-Co(1)-N(1)	121.76(9)	O(2A)-Co(1)-N(5)	96.95(8)	O(4)-Co(1)-N(1)	99.81(9)
N(1)-Co(1)-O(3)	86.62(8)	N(5)-Co(1)-O(4)	130.40(9)	N(5)-Co(1)-N(1)	113.69(11)
N(4B)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(5)	92.45(11)	N(4B)-Co(1)-N(1)	178.93(12)
N(1)-Co(1)-O(2)	90.39(11)	N(1)-Co(1)-O(1)	88.76(10)	N(1)-Co(1)-O(5)	86.98(11)

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Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(1)	2.1176(19)	Co(1)-O(1A)	2.1176(19)	Co(1)-N(1)	2.104(2)
Co(1)-N(1A)	2.104(2)	Co(1)-O(2)	2.1405(17)	Co(1)-N(2A)	2.1406(17)
Angle	(°)	Angle	(°)	Angle	(°)
N(1)-Co(1)-N(1A)	180.0	N(1)-Co(1)-O(1)	87.76(8)	N(1)-Co(1)-O(1A)	92.24(8)

N(1A)-Co(1)-O(1A)	92.24(9)	N(1A)-Co(1)-O(1)	87.76(8)	O(1)-Co(1)-O(1A)	180.0
N(1)-Co(1)-O(2)	89.23(8)	N(1)-Co(1)-O(2A)	90.77(8)	O(1)-Co(1)-O(2)	88.17(7)
O(1)-Co(1)-O(2A)	91.83(7)	N(1)-Co(1)-O(2)	90.775(8)	N(1)-Co(1)-O(2A)	89.23(8)
O(1A)-Co(1)-O(2)	91.83(7)	O(1A)-Co(1)-O(2A)	88.17(7)	O(2)-Co(1)-O(2A)	180.0

Symmetry code:

- 1 A: 1-x, -y, -z; B: 2-x, 1-y, 1-z; C: -1+x, -1+y, +z; D: 1-x, -y, 1-z.
- A: -x+1/2, y-1/2, -z+1/2.
- A: -x+3/2, y+1/2, z; B: -x+3/2, y-1/2, z.
- A: x-1/2, -y+1/2, z-1/2; B: x, y-1, z; C: x+1/2, -y+1/2, +z; D: x, y+1, z.
- A: x-1, y-1, z; B: -x-1, -y, -z+2; C: x+1, y+1, z.
- A: x-1/2, -y+1/2, z-1/2; B: x, y-1, z; C: x+1/2, -y+1/2, +z; D: x, y+1, z.