Supporting Information

Transfer and Control of Molecular Chirality in the 1:2 Host-Guest Supramolecular Complex Consisting of Mg(II) bisporphyrin and Chiral Diols: Effect of H-bonding on Rationalization of Chirality

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Instrumentation

Elemental (C, H, and N) analyses were performed on a CE-440 elemental analyzer. ¹H NMR spectra were recorded on a JEOL 500 MHz instrument. The residual ¹H resonances of thesolvents were used as a secondary reference. UV-vis and CD-spectra were recorded on a Perkin-Elmer UV-vis and a JASCO J-815 spectrometer, respectively. ESI-MS spectra were recorded on a waters Micromass Quattro Microtriple quadrapole mass spectrometer.

X-ray Structure Solution and Refinement. Single-crystal X-ray data were collected at 100 K on a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low temperature apparatus and intensity data were collected using graphite-monochromated Mo K α radiation (λ = 0.71073 Å). The data integration and reduction were processed with SAINT software.¹ An absorption correction was applied.² The structure was solved by the direct method using SHELXS-97 and was refined on F2 by full-matrix least-squares technique using the SHELXL-2014 program package.³ Non-hydrogen atoms were refined anisotropically. The protons of the diol guest substrate were directly located in the difference Fourier maps. The other hydrogen atoms were included in calculated positions. In the refinement, hydrogens were treated as riding atoms using SHELXL default parameters.

Computational details.

DFT calculations have been carried out by employing a B3LYP hybrid functional using the Gaussian 09, revision B.01, package.⁴ The method used was Becke's three parameter hybrid exchange functional,⁵ the nonlocal correlation provided by the Lee, Yang, and Parr expression,⁶ and Vosko, Wilk, and Nussair 1980 correlation functional (III) for local correction. The basis set were LANL2DZ for Mg and S and 6-31G+(d, p) for C, N, O, and H. Full geometry optimizations of all the complexes were carried out in dichloromethane taking the coordinates from the crystal structure of $1 \cdot (L^2)_2$. Dispersion corrections were not implemented as the increased attractive forces led to unreasonable porphyrin ring distances.

Experimental:

Materials:

The free base ligand 4,6-bis[5-(2,8,13,17-tetraethyl-3,7,12,18-tetramethylporphyrinyl)]dibenzothiophene has been synthesized following the reported procedure.⁷ Magnesium ion was inserted into free bisporphyrin by adding MgBr₂.OEt₂ to its anhydrous dichloromethane solution and subsequent stirring in presence of aliquot of distilled triethylamine for 1 hour under N₂ atmosphere.⁸ Pure dark reddish solid, 4,6-bis[Mg(II)-5-(3,7,13,17-tetraethyl-2,6,12,16-tetramethylporphyrinyl)]dibenzothiophene, **1** was obtained in excellent yield upon chromatographic purification using dichloromethane/acetone (1:1) as eluant. Enantiomerically pure chiral alcohols have been purchased from Sigma-Aldrich. Reagents and solvents are purchased from commercial sources and purified by standard procedures before use.

Synthesis of 1

50 mg (0.044 mmol) of the free base form of **1** was taken in 20 mL of anhydrous dichloromethane. 250 μ L of anhydrous triethylamine followed by MgBr₂.OEt₂ (227 mg, 0.88 mmol) were added to it, and stirred under N₂ atmosphere at room temperature for 1 hour. 50 mL of anhydrous dichloromethane was added to the reaction mixture and washed with distilled water once. The solvent was dried over anhydrous Na₂SO₄, filtered and evaporated to dryness. Column chromatography was done over basic alumina using dry CH₂Cl₂: Acetone(1:1) as eluant. Yield 36 mg (69%). Anal. Calcd (found): C, 77.21 (77.38); H, 6.48 (6.61); N, 9.47 (9.59). UV-vis (Dichloromethane) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 407 (3.97 × 10⁵), 421^{sh} (1.32 × 10⁵), 547 (2.22 ×

10⁴), 582 (1.56 × 10⁴). ¹H NMR (CDCl₃, 295K): δ, 9.68 (*s*, 4H, 10,20-meso-*H*); 9.63 (*s*, 2H, 15-meso-*H*); 8.79 (*d*, 2H, Ar-*H*); 8.02 (*d*, 2H, Ar-*H*); 7.96 (*t*, 2H, Ar-H); 3.83 (*m*, 16H , -C*H*₂); 3.32 (*s*, 12H, -C*H*₃); 2.25 (*s*, 12H, -C*H*₃); 1.58 (*t*, 12H, -C*H*₃); 1.48 (*t*, 12H, -C*H*₃) ppm. ESI-MS: *m*/*z* 1180.5672 ([M]⁺).

Synthesis of 1•L¹

Compound **1** (50 mg, 0.042 mmol) was dissolved in CH₂Cl₂ (5 mL). (2*R*, 3*R*)-2,3 butanediol (L²) (4.5 mg, 0.05mmol) was added to it and stirred for about 30 min. The solution obtained was then filtered off to remove any solid residue and carefully layered with acetonitrile at room temperature. On standing for 6-7 days reddish solid precipitated out, which was then isolated by filtration, washed well with n-hexane, and dried well in vacuum. Anal. Calcd (found): C, 75.52 (75.61); H, 6.81 (6.89); N, 8.80 (8.93). UV-vis (CH₂Cl₂) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 406 (3.46 × 10⁵), 420^{sh} (1.16 x 10⁵), 546 (2.45 × 10⁴), 583 (1.42 × 10⁴). ¹H NMR (CDCl₃, 295K): δ , 9.67 (*s*, 2H, 10-meso-*H*); 9.63 (*s*, 2H, 15-meso-*H*); 9.56 (*s*, 2H, 20-meso-*H*); 8.79 (*d*, 2H, Ar-*H*); 8.15 (*d*, 2H, Ar-*H*); 8.00 (*t*, 2H, Ar-*H*); 3.80 (*m*, 16H, -CH₂); 3.39 (*s*, 6H, -CH₃); 3.31 (*s*, 6H, -CH₃); 2.32 (*s*, 6H, -CH₃); 2.27 (*s*, 6H, -CH₃); 1.62 (*m*, 24H, -CH₃); -2.15 (*s*, 2H, -CH); -3.10 (*s*, 6H, -CH₃), -3.25 (*br*, 2H, -OH), ppm. ESI-MS: *m/z* 1270.6175 ([**1**•L²]⁺).

Synthesis of 1•(L²)₂

Compound **1** (50 mg, 0.042 mmol) was dissolved in CH₂Cl₂ (5 mL). (1*S*, 2*S*, 3*R*, 5*S*)-2,3pinanediol (L³) (17.0 mg, 0.1 mmol) was added to it and stirred for about 30 min. The solution obtained was then filtered off to remove any solid residue and carefully layered with acetonitrile at room temperature. On standing for 6-7 days reddish solid precipitated out, which was then isolated by filtration, washed well with n-hexane, and dried well in vacuum. Anal. Calcd (found): C, 75.72 (75.83); H, 7.41 (7.50); N, 7.35 (7.39). UV-vis (CHCl₃) [λ_{max} , nm (ε , M⁻¹ cm⁻¹)]: 409 (4.31 × 10⁵), 422^{sh} (1.36 × 10⁵), 548 (2.26 × 10⁴), 580 (1.45 × 10⁴). ¹H NMR (CDCl₃, 295 K): δ , 9.79 (*s*, 2H, 10-meso-*H*); 9.67 (*s*, 2H, 15-meso-*H*); 9.62 (*s*, 2H, 20-meso-*H*); 8.81 (*d*, 2H, Ar-*H*); 8.06 (*d*, 2H, Ar-*H*); 7.99 (*t*, 2H, Ar-*H*); 3.82 (*m*, 16H , -C*H*₂); 3.38 (*s*, 6H, -C*H*₃); 3.34 (*s*, 6H, -C*H*₃); 2.29 (*s*, 6H, -C*H*₃); 2.27 (*s*, 6H, -C*H*₃); 1.66 (*m*, 24H, -C*H*₃); 0.72 (*br*, 18H, -C*H*₃, L³-*H*); 0.45 (*br*, 8H, L³-*H*), -1.00 (*br*, 8H, L³-*H*), -1.82 (*br*, 2H, -O*H*, L³), ppm. ESI-MS: *m*/*z* 1521.8412 ([1•(L³)₂+H]⁺).

References

- (1) SAINT+, 6.02 ed., Bruker AXS, Madison, WI, 1999.
- (2) Sheldrick, G.M. SADABS 2.0, 2000.
- (3) Sheldrick, G. M. *SHELXL-2014: Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, **2014**.
- (4) Frisch, M.J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.
- (5) Becke, A. D. J. Chem. Phys. 1993, 98, 5648.
- (6) Lee, C.; Yang, W.; Parr, R. G. Phys. Rev. B. 1988, 37, 785.
- (7) Faure, S.; Stern, C.; Guilard, R.; Harvey, P. D. J. Am. Chem. Soc. 2004, 126, 1253.
- (8) Lintuluto, J. M.; Borovkov, V.V.; Inoue, Y. J. Am. Chem. Soc. 2002, 124, 13676.



Figure S1. UV-visible (in CH_2Cl_2 at 295 K) spectral change of **1** (at 3 x 10⁻⁶ M) upon addition of L^1 (2*R*, 3*R*)-2,3 butanediol as the host-guest molar ratio change from (A) 1:0 to 1:19 and (B) 1:50 to 860. Inset shows the expanded Soret band region.



Figure S2. UV-visible (in CH_2Cl_2 at 295 K) spectral change of **1** (at 3 x 10⁻⁶ M) upon gradual addition of L⁴, (*S*)-2-butanol as the host-guest ratio changes from 1:0 to 1:4300. Inset shows the expanded Soret band region.



Figure S3. UV-visible (in CH_2Cl_2 at 295 K) spectral change of **1** (at 3 x 10⁻⁶ M) upon gradual addition of L⁵, (1*S*)-borneol as the host-guest ratio changes from 1:0 to 1:7500. Inset shows the expanded Soret band region.



Figure S4. UV-visible (in CH_2Cl_2 at 295 K) spectral change of **1** (at 3 x 10⁻⁶ M) upon gradual addition of L⁶, (1*S*, 2*R*, 5*S*)-1-menthol as the host-guest ratio changes from 1:0 to 1:11300. Inset shows the expanded Soret band region.



Figure S5. Job's plot establishing the 1:1 stoichiometry for the binding between 1 and L^1 at a total concentration of 3×10^{-6} M in CH₂Cl₂ at 295 K (A) UV-vis absorbance change monitored at 407 nm, (B) CD amplitude vs. Host 1 mole fraction.



Figure S6. Isotopic distribution pattern (A) theoretical and (B) experimental of ESI-MS of $[1^{+}L^{1}]^{+}$.



Figure S7. Isotopic distribution pattern (A) theoretical and (B) experimental of ESI-MS of $[1\cdot(L^1)_2 + 2H]^+$.



Figure S8. Job's plot establishing the 1:2 stoichiometry for the binding between 1 and L^2 at a total concentration of 3×10^{-6} M in CH₂Cl₂ at 295 K (A) UV-vis absorbance change monitored at 409 nm, (B) CD amplitude vs. Host 1 mole fraction.



Figure S9. Diagram illustrating the packing of $1 \cdot (L^2)_2$ in the unit cell (H atoms have been omitted for clarity).



Figure S10. ¹H NMR spectra in CDCl₃ at 295 K of (A) **1** (7 mM), (B) after addition of 1.0 equivalent of L^1 to **1**, and (C) L^1 .



Figure S11. ¹H NMR spectra in CDCl₃ at 295 K of (A) **1**, (B) crystals of $1 \cdot (L^2)_2$ and (C) L^2 at 7 mM concentration. Inset shows the proton numbering scheme of L^2 .



Figure S12. (A) CD and UV-visible spectral changes upon addition of (2R, 3R)-2,3-butanediol (L¹) to the CH₂Cl₂ solution of **1** (3 × 10⁻⁶ M) at 295 K as the host: guest molar ratio changes from 1:0 to 1:843. (B) CD amplitude change.



Figure S13. (A) Calculated CD spectra of (red) **1**, (blue) $1 \cdot L^1$, (brown) $1 \cdot (L^1)_2$ and observed CD spectra of (black) $1 \cdot L^1$, (green) $1 \cdot (L^1)_2$. (B) Fits of CD titration data of $1(3 \times 10^{-6} \text{ M})$ with L^1 at selected wavelengths of 406 and 416 nm. (C) Species distribution plots of **1**, $1 \cdot L^1$ and $1 \cdot (L^1)_2$ complexes.



Figure S14. (A) CD and UV-visible spectral changes upon addition of (1*S*, 2*S*, 3*R*, 5*S*)-2,3pinanediol (L²) to the CH₂Cl₂ solution of **1** (3×10^{-6} M) at 295 K as the host: guest molar ratio changes from 1:0 to 1:354. (B) CD amplitude change.



Figure S15. (A) Calculated CD spectra of (red) **1**, (brown) $1 \cdot (L^2)_2$ and (green) observed CD spectra of $1 \cdot (L^2)_2$. (B) Fits of CD titration data of $1(3 \times 10^{-6} \text{ M})$ with L^2 at selected wavelengths of 407 and 418 nm. (C) Species distribution plots of **1**, $1 \cdot L^2$ and $1 \cdot (L^2)_2$ complexes.



Figure S16. (A) CD and UV-visible spectral changes upon addition of (1*R*, 2*R*, 3*S*, 5*R*)-2,3pinanediol (L³) to the CH₂Cl₂ solution of **1** (3×10^{-6} M) at 295 K as the host:guest molar ratio changes from 1:0 to 1:345. (B) CD amplitude change.



Figure S17. (A) Calculated CD spectra of (red) **1**, (green) $1 \cdot (L^3)_2$ and (brown) observed CD spectra of $1 \cdot (L^3)_2$. (B) Fits of CD titration data of $1(3 \times 10^{-6} \text{ M})$ with L^3 at selected wavelengths of 407 and 419 nm. (C) Species distribution plots of **1**, $1 \cdot L^3$ and $1 \cdot (L^3)_2$ complexes.



Figure S18. (A) Calculated UV-visible spectra of **1** (red), $1 \cdot L^1$ (blue) and $1 \cdot (L^1)_2$ (brown). Green line represents the observed UV-visible spectra of **1**. (B) Fits of absorbance data at selected wavelength of 407 nm. (C) Species distribution plots of **1**, $1 \cdot L^1$ and $1 \cdot (L^1)_2$ complexes.



Figure S19. (A) Calculated UV-visible spectra of **1** (red) and $1 \cdot (L^2)_2$ (blue). Green line represents the observed UV-visible spectra of **1**. (B) Fits of absorbance data at selected wavelength of 409 nm. (C) Species distribution plots of **1**, $1 \cdot L^2$ and $1 \cdot (L^2)_2$ complexes.



Figure S20. CD spectral change of **1** (3×10^{-6} M) in CH₂Cl₂ at 295 K upon addition of 1 equivalent of L² (red line), 1 equivalent of L² + 1 equivalent of L³ (green line), and 1 equivalent of L² + 250 equivalent of L³ (blue line).



Figure S21. Solid state UV-visible (bottom) and CD (top) spectra of $1 \cdot (L^2)_2$ in KBr matrix at 295 K.



Figure S22. CD and UV-visible spectral change of $1 (3 \times 10^{-6} \text{ M})$ in CH₂Cl₂ at 295 K upon addition of (*S*)-2-butanol (L⁴) as the host-guest molar ratio changes 1:0 to 1:4300.



Figure S23. CD and UV-visible spectral change of $1 (3 \times 10^{-6} \text{ M})$ in CH₂Cl₂ at 295 K upon gradual addition of (1*S*)-borneol (L⁵) as the host-guest ratio changes from 1:0 to 1:7500



Figure S24. CD and UV-visible spectral change of $1 (3 \times 10^{-6} \text{ M})$ in CH₂Cl₂ at 295 K upon addition of various amount of (1*S*, 2*R*, 5*S*)-1-menthol (L⁶) as the host-guest ratio changes from 1:0 to 1:11300.



Figure S25. Relative energy of DFT-optimized *endo-endo*, *exo-endo* and *exo-exo* conformers of $1 \cdot (L^2)_2$.



Figure S26. Relative energy of DFT-optimized *exo-endo*, *exo-exo* and *endo-endo* conformers of $1 \cdot (L^2)_2$ where unbound –OH of L^2 is replaced manually by –CH₃.



Figure S27. Relative energy of DFT-optimized *exo-endo*, *exo-exo* and *endo-endo* conformers of $1 \cdot (L^2)_2$ where unbound –OH of L^2 is replaced manually by –SH.

Compounds	FC ^a	SC ^a	$A_{cal}{}^b$	Binding Constant	FC ^a	SC ^a	$A_{\rm cal}{}^{\rm b}$	Binding
			[cm ⁻¹ M ⁻¹]	$K_1 (\mathrm{M}^{-1})^{c,d}$			[cm ⁻¹ M ⁻¹]	Constant
								$K_2 ({ m M}^{-1})^{c,d}$
	1:1 comple	ex, CD data			1:2 comple	ex, CD data		
	λ (nm) [Δ	ε, cm ⁻¹ M ⁻¹]			λ (nm) [$\Delta \epsilon$	c, cm ⁻¹ M ⁻¹]		
1 •L ¹	416[35]	405[-23]	58	$3.5 \pm 0.2 \times 10^5 \mathrm{M}^{-1}$	416[-118]	406[70]	-188	$2.4 \pm 0.3 \times 10^3 \text{ M}^{-1}$
				$[2.6\pm 0.1\times 10^5~M^{1}]$				$[2.5\pm0.2\times10^3~M^{1}]$
$1 \cdot (L^2)_2$				$6.3\pm 0.2\times 10^{4}M^{1}$	418[-117]	407[98]	-215	$2.5\pm 0.1\times 10^{4}M^{1}$
				$[5.6\pm 0.1\times 10^4M^{1}]$				$[2.2\pm0.2\times10^4~M^{1}]$
$1 \cdot (L^3)_2$				$6.6\pm 0.1\times 10^4M^{-1}$	419[118]	407[-101]	219	$2.7\pm 0.1\times 10^4M^{1}$
				$[5.8\pm0.2\times10^4M^{1}]$				$[2.4\pm0.1\times10^4M^{1}]$

Table S1. Calculated CD Spectral Data and Binding Constants of the Complexes at 295 K.

^aFC: 1st Cotton effect; ^aSC: 2nd Cotton effect. ^bA: total amplitude in M⁻¹ cm⁻¹; $A = |\Delta \varepsilon_1 - \Delta \varepsilon_2|$ ^cCalculated from CD spectral measurement. ^dValue shown within the bracket are calculated from UV-visible spectral measurement.

Table S2.	Selected Bond Lengths (Å) and Angles (deg) for DFT-optimized conformers exo-
endo, exo-	<i>exo</i> and <i>endo-endo</i> of $1 \cdot (L^3)_2$

Bond Lengths (Å)	exo-endo	exo-exo	endo-endo
Mg(1)-N(1)	2.119	2.101	2.102
Mg(1)-N(2)	2.105	2.108	2.102
Mg(1)-N(3)	2.101	2.105	2.108
Mg(1)-N(4)	2.099	2.100	2.100
Mg(1)-O(1)	2.069	2.080	2.109
Mg(2)-N(5)	2.103	2.105	2.109

Mg(2)-N(6)	2.116	2.102	2.116
Mg(2)-N(7)	2.114	2.106	2.112
Mg(2)-N(8)	2.110	2.099	2.105
Mg(2)-O(3)	2.081	2.080	2.098
Bond Angles (deg)			
N(1)-Mg(1)-N(2)	89.71	90.47	90.10
N(1)-Mg(1)-N(3)	159.47	162.77	160.97
N(1)-Mg(1)-N(4)	86.46	86.90	87.12
N(2)-Mg(1)-N(3)	87.12	86.84	87.29
N(2)-Mg(1)-N(4)	161.94	162.25	163.13
N(3)-Mg(1)-N(4)	90.30	90.50	89.93
N(5)-Mg(2)-N(6)	89.68	90.36	89.43
N(5)-Mg(2)-N(7)	160.17	161.69	159.19
N(5)-Mg(2)-N(8)	86.76	86.91	86.69
N(6)-Mg(2)-N(7)	86.52	87.16	86.64
N(6)-Mg(2)-N(8)	158.05	163.64	158.82
N(7)-Mg(2)-N(8)	89.52	90.38	89.63

Table S3. Selected Bond Lengths (Å) and Angles (deg) for DFT-optimized conformers *exo-endo*, *exo-exo* and *endo-endo* of $1^{\circ}(L^3)_2$ where unbound –OH of L^2 is replaced manually by – CH₃.

Bond Lengths (Å)	exo-endo	exo-exo	endo-endo
Mg(1)-N(1)	2.099	2.098	2.101
Mg(1)-N(2)	2.109	2.099	2.102
Mg(1)-N(3)	2.098	2.101	2.104
Mg(1)-N(4)	2.100	2.100	2.095
Mg(1)-O(1)	2.096	2.101	2.103
Mg(2)-N(5)	2.098	2.097	2.098
Mg(2)-N(6)	2.102	2.102	2.102
Mg(2)-N(7)	2.105	2.105	2.100
Mg(2)-N(8)	2.092	2.092	2.103
Mg(2)-O(3)	2.101	2.101	2.099
Bond Angles (deg)			
N(1)-Mg(1)-N(2)	90.18	90.80	90.04
N(1)-Mg(1)-N(3)	163.94	163.88	161.90
N(1)-Mg(1)-N(4)	87.03	86.90	87.32
N(2)-Mg(1)-N(3)	87.08	87.06	87.41
N(2)-Mg(1)-N(4)	161.21	163.54	163.48
N(3)-Mg(1)-N(4)	90.47	90.63	90.03
N(5)-Mg(2)-N(6)	90.53	90.64	90.26
N(5)-Mg(2)-N(7)	161.92	162.69	162.85
N(5)-Mg(2)-N(8)	87.24	87.25	86.90

N(6)-Mg(2)-N(7)	87.11	87.07	87.18
N(6)-Mg(2)-N(8)	165.24	165.16	162.54
N(7)-Mg(2)-N(8)	90.47	90.56	90.46

Table S4. Selected Bond Lengths (Å) and Angles (deg) for DFT-optimized conformers *exoendo*, *exo-exo* and *endo-endo* of $1^{\circ}(L^{3})_{2}$ where unbound –OH of L^{2} is replaced manually by –SH.

Bond Lengths (Å)	exo-endo	exo-exo	endo-endo
Mg(1)-N(1)	2.101	2.097	2.106
Mg(1)-N(2)	2.107	2.105	2.104
Mg(1)-N(3)	2.102	2.099	2.111
Mg(1)-N(4)	2.103	2.097	2.096
Mg(1)-O(1)	2.091	2.097	2.129
Mg(2)-N(5)	2.099	2.097	2.099
Mg(2)-N(6)	2.096	2.100	2.102
Mg(2)-N(7)	2.106	2.103	2.105
Mg(2)-N(8)	2.094	2.095	2.098
Mg(2)-O(3)	2.103	2.094	2.093
Bond Angles (deg)			
N(1)-Mg(1)-N(2)	89.91	90.69	90.28
N(1)-Mg(1)-N(3)	162.35	163.68	159.73
N(1)-Mg(1)-N(4)	87.02	86.99	86.70
N(2)-Mg(1)-N(3)	87.19	86.95	86.72
N(2)-Mg(1)-N(4)	161.22	163.31	161.38

N(3)-Mg(1)-N(4)	90.12	90.71	89.76
N(5)-Mg(2)-N(6)	90.58	90.70	90.16
N(5)-Mg(2)-N(7)	162.39	162.69	162.51
N(5)-Mg(2)-N(8)	87.20	87.09	87.35
N(6)-Mg(2)-N(7)	87.32	87.04	87.29
N(6)-Mg(2)-N(8)	165.20	164.84	163.30
N(7)-Mg(2)-N(8)	90.36	90.60	90.12