

## Supporting information

### 1 Magnetic equations

Independent parameters are  $\kappa$ ,  $\lambda$ ,  $v$ ,  $q$ , and  $p$ .

$$\Delta = v\kappa\lambda$$

$$Q = q\kappa\lambda$$

$$P = p\kappa\lambda$$

$$g_e = 2.0023$$

$$c_{11} = \frac{d_{11}}{\sqrt{d_{11}^2 + d_{12}^2 + d_{13}^2}}$$

$$c_{12} = \frac{d_{12}}{\sqrt{d_{11}^2 + d_{12}^2 + d_{13}^2}}$$

$$c_{13} = \frac{d_{13}}{\sqrt{d_{11}^2 + d_{12}^2 + d_{13}^2}}$$

$$c_{31} = \frac{d_{31}}{\sqrt{d_{31}^2 + d_{32}^2 + d_{33}^2}}$$

$$c_{32} = \frac{d_{32}}{\sqrt{d_{31}^2 + d_{32}^2 + d_{33}^2}}$$

$$c_{33} = \frac{d_{33}}{\sqrt{d_{31}^2 + d_{32}^2 + d_{33}^2}}$$

$$c_{41} = \frac{d_{41}}{\sqrt{d_{41}^2 + d_{42}^2 + d_{43}^2}}$$

$$c_{42} = \frac{d_{42}}{\sqrt{d_{41}^2 + d_{42}^2 + d_{43}^2}}$$

$$c_{43} = \frac{d_{43}}{\sqrt{d_{41}^2 + d_{42}^2 + d_{43}^2}}$$

$$c_{24} = \frac{d_{21}}{\sqrt{d_{21}^2 + d_{22}^2}}$$

$$c_{25} = \frac{d_{22}}{\sqrt{d_{21}^2 + d_{22}^2}}$$

$$c_{54} = \frac{d_{51}}{\sqrt{d_{51}^2 + d_{52}^2}}$$

$$c_{55} = \frac{d_{52}}{\sqrt{d_{51}^2 + d_{52}^2}}$$

$$d_{11} = \frac{3q}{6+3q-4v-ec1}$$

$$d_{12} = -1$$

$$d_{13} = \frac{6}{3+2v-ec1}$$

$$d_{31} = \frac{3q}{6+3q-4v-ec3}$$

$$d_{32} = -1$$

$$d_{33} = \frac{6}{3+2v-ec3}$$

$$d_{41} = \frac{3q}{6+3q-4v-ec4}$$

$$d_{42} = -1$$

$$d_{43} = \frac{6}{3+2v-ec4}$$

$$d_{21} = \frac{3\sqrt{6}}{-3+2v-ec2}$$

$$d_{22} = -1$$

$$d_{51} = \frac{3\sqrt{6}}{-3+2v-ec5}$$

$$d_{52} = -1$$

$$A = -36v^2 + 36qv - 36v - 36q^2 + 18q - 225$$

$$B = -432v^3 + 648qv^2 - 648v^2 + 648q^2v + 648qv + 1620v - 432q^3 + 324q^2 - 810q + 6750$$

$$ec1 = -2v + 2q + 1 - \frac{\sqrt[3]{B+\sqrt{4A^3+B^2}}}{3\sqrt[3]{2}} + \frac{\sqrt[3]{2}A}{3\sqrt[3]{B+\sqrt{4A^3+B^2}}}$$

$$ec2 = \frac{1}{2} \left( -2v + 6p - 3 - 3\sqrt{4v^2 - 8pv - 4v + 4p^2 + 4p + 25} \right)$$

$$ec3 = -2v + 2q + 1 + \frac{(1+i\sqrt{3})\sqrt[3]{B+\sqrt{4A^3+B^2}}}{6\sqrt[3]{2}} - \frac{(1-i\sqrt{3})A}{3\sqrt[3]{2}\sqrt[3]{B+\sqrt{4A^3+B^2}}}$$

$$ec4 = -2v + 2q + 1 + \frac{(1-i\sqrt{3})\sqrt[3]{B+\sqrt{4A^3+B^2}}}{6\sqrt[3]{2}} - \frac{(1+i\sqrt{3})A}{3\sqrt[3]{2}\sqrt[3]{B+\sqrt{4A^3+B^2}}}$$

$$ec5 = \frac{1}{2} \left( -2v + 6p - 3 + 3\sqrt{4v^2 - 8pv - 4v + 4p^2 + 4p + 25} \right)$$

$$\begin{aligned}
E_{\pm 1}^{(0)} &= c_{11}^2 \left( \frac{-2\Delta}{3} + \kappa\lambda + \frac{Q}{2} \right) + 2c_{11}c_{12} \left( \frac{Q}{2} \right) + c_{12}^2 \left( \frac{-2\Delta}{3} - \kappa\lambda + \frac{Q}{2} \right) + 2c_{12}c_{13}(\kappa\lambda) + c_{13}^2 \left( \frac{\Delta}{3} + \frac{\kappa\lambda}{2} \right) \\
E_{\pm 2}^{(0)} &= c_{24}^2 \left( \frac{\Delta}{3} - \frac{\kappa\lambda}{2} \right) + 2c_{24}c_{25} \left( \frac{\sqrt{6}\kappa\lambda}{2} \right) + c_{25}^2 \left( \frac{-2\Delta}{3} + P \right) \\
E_{\pm 3}^{(0)} &= c_{31}^2 \left( \frac{-2\Delta}{3} + \kappa\lambda + \frac{Q}{2} \right) + 2c_{31}c_{32} \left( \frac{Q}{2} \right) + c_{32}^2 \left( \frac{-2\Delta}{3} - \kappa\lambda + \frac{Q}{2} \right) + 2c_{32}c_{33}(\kappa\lambda) + c_{33}^2 \left( \frac{\Delta}{3} + \frac{\kappa\lambda}{2} \right) \\
E_{\pm 4}^{(0)} &= c_{41}^2 \left( \frac{-2\Delta}{3} + \kappa\lambda + \frac{Q}{2} \right) + 2c_{41}c_{42} \left( \frac{Q}{2} \right) + c_{42}^2 \left( \frac{-2\Delta}{3} - \kappa\lambda + \frac{Q}{2} \right) + 2c_{42}c_{43}(\kappa\lambda) + c_{43}^2 \left( \frac{\Delta}{3} + \frac{\kappa\lambda}{2} \right) \\
E_{\pm 5}^{(0)} &= c_{54}^2 \left( \frac{\Delta}{3} - \frac{\kappa\lambda}{2} \right) + 2c_{54}c_{55} \left( \frac{\sqrt{6}\kappa\lambda}{2} \right) + c_{55}^2 \left( \frac{-2\Delta}{3} + P \right) \\
E_{1,z}^{(1)} &= -E_{-1,z}^{(1)} = (c_{11}^2(2\kappa + g_e/2) + c_{12}^2(-2\kappa + g_e/2) + c_{13}^2(-\kappa - g_e/2)) \beta \\
E_{2,z}^{(1)} &= -E_{-2,z}^{(1)} = (c_{24}^2(\kappa - g_e/2) + c_{25}^2(g_e/2)) \beta \\
E_{3,z}^{(1)} &= -E_{-3,z}^{(1)} = (c_{31}^2(2\kappa + g_e/2) + c_{32}^2(-2\kappa + g_e/2) + c_{33}^2(-\kappa - g_e/2)) \beta \\
E_{4,z}^{(1)} &= -E_{-4,z}^{(1)} = (c_{41}^2(2\kappa + g_e/2) + c_{42}^2(-2\kappa + g_e/2) + c_{43}^2(-\kappa - g_e/2)) \beta \\
E_{5,z}^{(1)} &= -E_{-5,z}^{(1)} = (c_{54}^2(\kappa - g_e/2) + c_{55}^2(g_e/2)) \beta \\
E_{\pm 1,z}^{(2)} &= \left( \frac{(c_{11}c_{31}(2\kappa + g_e/2) + c_{12}c_{32}(-2\kappa + g_e/2) + c_{13}c_{33}(-\kappa - g_e/2))^2}{E_1^{(0)} - E_3^{(0)}} + \frac{(c_{11}c_{41}(2\kappa + g_e/2) + c_{12}c_{42}(-2\kappa + g_e/2) + c_{13}c_{43}(-\kappa - g_e/2))^2}{E_1^{(0)} - E_4^{(0)}} \right) \beta^2 \\
E_{\pm 2,z}^{(2)} &= \left( \frac{(c_{24}c_{54}(\kappa - g_e/2) + c_{25}c_{55}(g_e/2))^2}{E_2^{(0)} - E_5^{(0)}} \right) \beta^2 \\
E_{\pm 3,z}^{(2)} &= \left( \frac{(c_{11}c_{31}(2\kappa + g_e/2) + c_{12}c_{32}(-2\kappa + g_e/2) + c_{13}c_{33}(-\kappa - g_e/2))^2}{E_3^{(0)} - E_1^{(0)}} + \frac{(c_{31}c_{41}(2\kappa + g_e/2) + c_{32}c_{42}(-2\kappa + g_e/2) + c_{33}c_{43}(-\kappa - g_e/2))^2}{E_3^{(0)} - E_4^{(0)}} \right) \beta^2 \\
E_{\pm 4,z}^{(2)} &= \left( \frac{(c_{41}c_{31}(2\kappa + g_e/2) + c_{42}c_{32}(-2\kappa + g_e/2) + c_{43}c_{33}(-\kappa - g_e/2))^2}{E_4^{(0)} - E_3^{(0)}} + \frac{(c_{11}c_{41}(2\kappa + g_e/2) + c_{12}c_{42}(-2\kappa + g_e/2) + c_{13}c_{43}(-\kappa - g_e/2))^2}{E_4^{(0)} - E_1^{(0)}} \right) \beta^2 \\
E_{\pm 5,z}^{(2)} &= \left( \frac{(c_{24}c_{54}(\kappa - g_e/2) + c_{25}c_{55}(g_e/2))^2}{E_5^{(0)} - E_2^{(0)}} \right) \beta^2 \\
E_{1,x}^{(1)} &= -E_{-1,x}^{(1)} = (2c_{11}c_{12}(g_e/2) + 2c_{11}c_{13}(\kappa)) \beta \\
E_{2,x}^{(1)} &= -E_{-2,x}^{(1)} = \left( 2c_{24}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right) + c_{25}c_{25}(g_e/2) \right) \beta \\
E_{3,x}^{(1)} &= -E_{-3,x}^{(1)} = (2c_{31}c_{32}(g_e/2) + 2c_{31}c_{33}(\kappa)) \beta \\
E_{4,x}^{(1)} &= -E_{-4,x}^{(1)} = (2c_{41}c_{42}(g_e/2) + 2c_{41}c_{43}(\kappa)) \beta \\
E_{5,x}^{(1)} &= -E_{-5,x}^{(1)} = \left( 2c_{54}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right) + c_{55}c_{55}(g_e/2) \right) \beta \\
E_{\pm 1,x}^{(2)} &= \left( \frac{(c_{12}c_{24}\kappa + c_{13}c_{24}(g_e/2) + c_{13}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_1^{(0)} - E_2^{(0)}} + \frac{((c_{11}c_{32} + c_{12}c_{31})(g_e/2) + (c_{11}c_{33} + c_{13}c_{31})\kappa)^2}{E_1^{(0)} - E_3^{(0)}} + \right. \\
&\quad \left. \frac{((c_{11}c_{42} + c_{12}c_{41})(g_e/2) + (c_{11}c_{43} + c_{13}c_{41})\kappa)^2}{E_1^{(0)} - E_4^{(0)}} + \frac{(c_{12}c_{54}\kappa + c_{13}c_{54}(g_e/2) + c_{13}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_1^{(0)} - E_5^{(0)}} \right) \beta^2 \\
E_{\pm 2,x}^{(2)} &= \left( \frac{(c_{12}c_{24}\kappa + c_{13}c_{24}(g_e/2) + c_{13}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_2^{(0)} - E_1^{(0)}} + \frac{(c_{32}c_{24}\kappa + c_{33}c_{24}(g_e/2) + c_{33}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_2^{(0)} - E_3^{(0)}} + \right. \\
&\quad \left. \frac{(c_{42}c_{24}\kappa + c_{43}c_{24}(g_e/2) + c_{43}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_2^{(0)} - E_4^{(0)}} + \frac{(c_{25}c_{55}(g_e/2) + (c_{24}c_{55} + c_{25}c_{54}) \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_2^{(0)} - E_5^{(0)}} \right) \beta^2 \\
E_{\pm 3,x}^{(2)} &= \left( \frac{(c_{32}c_{24}\kappa + c_{33}c_{24}(g_e/2) + c_{33}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_3^{(0)} - E_2^{(0)}} + \frac{((c_{11}c_{32} + c_{12}c_{31})(g_e/2) + (c_{11}c_{33} + c_{13}c_{31})\kappa)^2}{E_3^{(0)} - E_1^{(0)}} + \right. \\
&\quad \left. \frac{((c_{31}c_{42} + c_{32}c_{41})(g_e/2) + (c_{31}c_{43} + c_{33}c_{41})\kappa)^2}{E_3^{(0)} - E_4^{(0)}} + \frac{(c_{32}c_{54}\kappa + c_{33}c_{54}(g_e/2) + c_{33}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_3^{(0)} - E_5^{(0)}} \right) \beta^2 \\
E_{\pm 4,x}^{(2)} &= \left( \frac{(c_{42}c_{24}\kappa + c_{43}c_{24}(g_e/2) + c_{43}c_{25} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_4^{(0)} - E_2^{(0)}} + \frac{((c_{41}c_{32} + c_{42}c_{31})(g_e/2) + (c_{41}c_{33} + c_{43}c_{31})\kappa)^2}{E_4^{(0)} - E_3^{(0)}} + \right. \\
&\quad \left. \frac{((c_{11}c_{42} + c_{12}c_{41})(g_e/2) + (c_{11}c_{43} + c_{13}c_{41})\kappa)^2}{E_4^{(0)} - E_1^{(0)}} + \frac{(c_{42}c_{54}\kappa + c_{43}c_{54}(g_e/2) + c_{43}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_4^{(0)} - E_5^{(0)}} \right) \beta^2 \\
E_{\pm 5,x}^{(2)} &= \left( \frac{(c_{12}c_{54}\kappa + c_{13}c_{54}(g_e/2) + c_{13}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_5^{(0)} - E_1^{(0)}} + \frac{(c_{32}c_{54}\kappa + c_{33}c_{54}(g_e/2) + c_{33}c_{55} \left( \frac{\sqrt{6}}{2} \kappa \right))^2}{E_5^{(0)} - E_3^{(0)}} + \right.
\end{aligned}$$

$$\left( \frac{(c_{42}c_{54}\kappa + c_{43}c_{54}(g_e/2) + c_{43}c_{55}(\frac{\sqrt{6}}{2}\kappa))^2}{E_5^{(0)} - E_4^{(0)}} + \frac{(c_{25}c_{55}(g_e/2) + (c_{24}c_{55} + c_{25}c_{54})(\frac{\sqrt{6}}{2}\kappa))^2}{E_5^{(0)} - E_2^{(0)}} \right) \beta^2$$

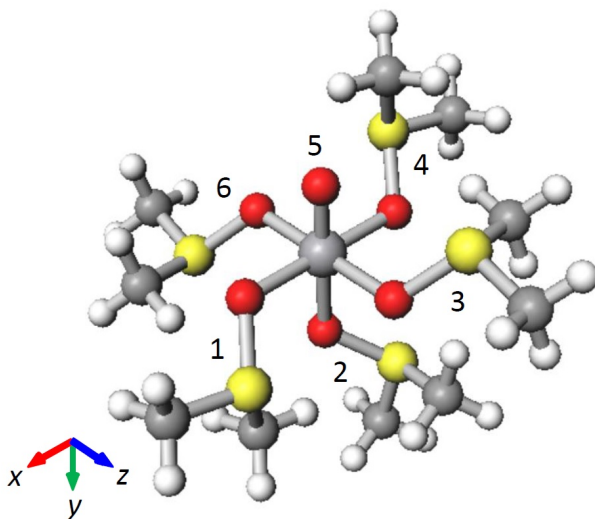
$$\chi_A = \frac{\chi_z + 2\chi_x}{3}$$

$$\chi_z(x) = \frac{N \sum_n (-E_{n,z(x)}^{(1)} - 2E_{n,z(x)}^{(2)} H_{z(x)}) \exp\left[\frac{-E_{n,z(x)}}{kT}\right]}{H_{z(x)} \sum_n \exp\left[\frac{-E_{n,z(x)}}{kT}\right]}$$

$$M_{av} = \sum_{j=1}^m M\left(\frac{(j-\frac{45}{m})\pi}{180}\right) \left[\cos\frac{(j-1)\pi}{180} - \cos\frac{j\pi}{180}\right]$$

$$M(\theta) = \frac{N \sum_n (-E_{n,\theta}^{(1)} - 2E_{n,\theta}^{(2)} H_\theta) \exp\left[\frac{-E_{n,\theta}}{kT}\right]}{\sum_n \exp\left[\frac{-E_{n,\theta}}{kT}\right]}$$

## 2 Conformer codes



**Fig. S1.** An example of a conformer with a numbering system.  
The numbering order is  $x, y, z, -x, -y, -z$ .

Conformer codes are based on the reference [H. Sakiyama and K. Waki, *J. Math. Chem.*, 2017, **55**, 1360].

**Table S1.** Conformers of [MX(ABC)<sub>5</sub>] complexes with L5-B35 core

Code	Dihedral angles (°) of M-A-B-C units
L5-B35-1	[180,180,180,180,-,180]
L5-B35-2	[300,180,180,180,-,180]
L5-B35-3	[60,180,180,180,-,180]
L5-B35-4	[180,300,180,180,-,180]
L5-B35-5	[300,300,180,180,-,180]
L5-B35-6	[60,300,180,180,-,180]
L5-B35-7	[180,60,180,180,-,180]
L5-B35-8	[300,60,180,180,-,180]
L5-B35-9	[60,60,180,180,-,180]
L5-B35-10	[180,180,300,180,-,180]
L5-B35-11	[300,180,300,180,-,180]
L5-B35-12	[60,180,300,180,-,180]
L5-B35-13	[180,300,300,180,-,180]
L5-B35-14	[300,300,300,180,-,180]
L5-B35-15	[60,300,300,180,-,180]
L5-B35-16	[180,60,300,180,-,180]
L5-B35-17	[300,60,300,180,-,180]
L5-B35-18	[60,60,300,180,-,180]
L5-B35-19	[180,180,60,180,-,180]
L5-B35-20	[300,180,60,180,-,180]
L5-B35-21	[60,180,60,180,-,180]
L5-B35-22	[180,300,60,180,-,180]
L5-B35-23	[300,300,60,180,-,180]
L5-B35-24	[60,300,60,180,-,180]
L5-B35-25	[180,60,60,180,-,180]
L5-B35-26	[300,60,60,180,-,180]
1 L5-B35-27	[60,60,60,180,-,180]
L5-B35-28	[180,180,180,300,-,180]
L5-B35-29	[300,180,180,300,-,180]
L5-B35-30	[60,180,180,300,-,180]
L5-B35-31	[180,300,180,300,-,180]
L5-B35-32	[300,300,180,300,-,180]
L5-B35-33	[60,300,180,300,-,180]
L5-B35-34	[180,60,180,300,-,180]
L5-B35-35	[300,60,180,300,-,180]
L5-B35-36	[60,60,180,300,-,180]
L5-B35-37	[180,180,300,300,-,180]
L5-B35-38	[300,180,300,300,-,180]
L5-B35-39	[60,180,300,300,-,180]
L5-B35-40	[180,300,300,300,-,180]
L5-B35-41	[300,300,300,300,-,180]
L5-B35-42	[60,300,300,300,-,180]
L5-B35-43	[180,60,300,300,-,180]
L5-B35-44	[300,60,300,300,-,180]
L5-B35-45	[60,60,300,300,-,180]
L5-B35-46	[180,180,60,300,-,180]
L5-B35-47	[300,180,60,300,-,180]
L5-B35-48	[60,180,60,300,-,180]
L5-B35-49	[180,300,60,300,-,180]
L5-B35-50	[300,300,60,300,-,180]
L5-B35-51	[60,300,60,300,-,180]
L5-B35-52	[180,60,60,300,-,180]
L5-B35-53	[300,60,60,300,-,180]
L5-B35-54	[60,60,60,300,-,180]
L5-B35-55	[180,180,180,60,-,180]

Code	Dihedral angles (°) of M-A-B-C units
L5-B35-56	[300,180,180,60,-,180]
L5-B35-57	[60,180,180,60,-,180]
L5-B35-58	[180,300,180,60,-,180]
L5-B35-59	[300,300,180,60,-,180]
L5-B35-60	[60,300,180,60,-,180]
L5-B35-61	[180,60,180,60,-,180]
L5-B35-62	[300,60,180,60,-,180]
L5-B35-63	[60,60,180,60,-,180]
L5-B35-64	[180,180,300,60,-,180]
L5-B35-65	[300,180,300,60,-,180]
L5-B35-66	[60,180,300,60,-,180]
L5-B35-67	[180,300,300,60,-,180]
L5-B35-68	[300,300,300,60,-,180]
L5-B35-69	[60,300,300,60,-,180]
L5-B35-70	[180,60,300,60,-,180]
L5-B35-71	[300,60,300,60,-,180]
L5-B35-72	[60,60,300,60,-,180]
L5-B35-73	[180,180,60,60,-,180]
L5-B35-74	[300,180,60,60,-,180]
L5-B35-75	[60,180,60,60,-,180]
L5-B35-76	[180,300,60,60,-,180]
L5-B35-77	[300,300,60,60,-,180]
L5-B35-78	[60,300,60,60,-,180]
L5-B35-79	[180,60,60,60,-,180]
L5-B35-80	[300,60,60,60,-,180]
L5-B35-81	[60,60,60,60,-,180]
L5-B35-82	[180,180,180,180,-,300]
L5-B35-83	[300,180,180,180,-,300]
L5-B35-84	[60,180,180,180,-,300]
L5-B35-85	[180,300,180,180,-,300]
L5-B35-86	[300,300,180,180,-,300]
L5-B35-87	[60,300,180,180,-,300]
L5-B35-88	[180,60,180,180,-,300]
L5-B35-89	[300,60,180,180,-,300]
L5-B35-90	[60,60,180,180,-,300]
L5-B35-91	[180,180,300,180,-,300]
L5-B35-92	[300,180,300,180,-,300]
L5-B35-93	[60,180,300,180,-,300]
L5-B35-94	[180,300,300,180,-,300]
L5-B35-95	[300,300,300,180,-,300]
L5-B35-96	[60,300,300,180,-,300]
L5-B35-97	[180,60,300,180,-,300]
L5-B35-98	[300,60,300,180,-,300]
L5-B35-99	[60,60,300,180,-,300]
L5-B35-100	[180,180,60,180,-,300]
L5-B35-101	[300,180,60,180,-,300]
L5-B35-102	[60,180,60,180,-,300]
L5-B35-103	[180,300,60,180,-,300]
L5-B35-104	[300,300,60,180,-,300]
L5-B35-105	[60,300,60,180,-,300]
L5-B35-106	[180,60,60,180,-,300]
L5-B35-107	[300,60,60,180,-,300]
L5-B35-108	[60,60,60,180,-,300]
L5-B35-109	[180,180,180,300,-,300]
L5-B35-110	[300,180,180,300,-,300]
L5-B35-111	[60,180,180,300,-,300]
L5-B35-112	[180,300,180,300,-,300]

Code	Dihedral angles ( $^{\circ}$ ) of M-A-B-C units
L5-B35-113	[300,300,180,300,-,300]
L5-B35-114	[60,300,180,300,-,300]
L5-B35-115	[180,60,180,300,-,300]
L5-B35-116	[300,60,180,300,-,300]
L5-B35-117	[60,60,180,300,-,300]
L5-B35-118	[180,180,300,300,-,300]
L5-B35-119	[300,180,300,300,-,300]
L5-B35-120	[60,180,300,300,-,300]
L5-B35-121	[180,300,300,300,-,300]
L5-B35-122	[300,300,300,300,-,300]
L5-B35-123	[60,300,300,300,-,300]
L5-B35-124	[180,60,300,300,-,300]
L5-B35-125	[300,60,300,300,-,300]
L5-B35-126	[60,60,300,300,-,300]
L5-B35-127	[180,180,60,300,-,300]
L5-B35-128	[300,180,60,300,-,300]
L5-B35-129	[60,180,60,300,-,300]
L5-B35-130	[180,300,60,300,-,300]
L5-B35-131	[300,300,60,300,-,300]
L5-B35-132	[60,300,60,300,-,300]
L5-B35-133	[180,60,60,300,-,300]
L5-B35-134	[300,60,60,300,-,300]
L5-B35-135	[60,60,60,300,-,300]
L5-B35-136	[180,180,180,60,-,300]
L5-B35-137	[300,180,180,60,-,300]
L5-B35-138	[60,180,180,60,-,300]
L5-B35-139	[180,300,180,60,-,300]
L5-B35-140	[300,300,180,60,-,300]
L5-B35-141	[60,300,180,60,-,300]
L5-B35-142	[180,60,180,60,-,300]
L5-B35-143	[300,60,180,60,-,300]
L5-B35-144	[60,60,180,60,-,300]
L5-B35-145	[180,180,300,60,-,300]
L5-B35-146	[300,180,300,60,-,300]
L5-B35-147	[60,180,300,60,-,300]
L5-B35-148	[180,300,300,60,-,300]
L5-B35-149	[300,300,300,60,-,300]
L5-B35-150	[60,300,300,60,-,300]
L5-B35-151	[180,60,300,60,-,300]
L5-B35-152	[300,60,300,60,-,300]
L5-B35-153	[60,60,300,60,-,300]
L5-B35-154	[180,180,60,60,-,300]
L5-B35-155	[300,180,60,60,-,300]
L5-B35-156	[60,180,60,60,-,300]
L5-B35-157	[180,300,60,60,-,300]
L5-B35-158	[300,300,60,60,-,300]
L5-B35-159	[60,300,60,60,-,300]
L5-B35-160	[180,60,60,60,-,300]
L5-B35-161	[300,60,60,60,-,300]
L5-B35-162	[60,60,60,60,-,300]
L5-B35-163	[180,180,180,180,-,60]
L5-B35-164	[300,180,180,180,-,60]
L5-B35-165	[60,180,180,180,-,60]
L5-B35-166	[180,300,180,180,-,60]
L5-B35-167	[300,300,180,180,-,60]
L5-B35-168	[60,300,180,180,-,60]
L5-B35-169	[180,60,180,180,-,60]
L5-B35-170	[300,60,180,180,-,60]

Code	Dihedral angles ( $^{\circ}$ ) of M-A-B-C units
L5-B35-171	[60,60,180,180,-,60]
L5-B35-172	[180,180,300,180,-,60]
L5-B35-173	[300,180,300,180,-,60]
L5-B35-174	[60,180,300,180,-,60]
L5-B35-175	[180,300,300,180,-,60]
L5-B35-176	[300,300,300,180,-,60]
L5-B35-177	[60,300,300,180,-,60]
L5-B35-178	[180,60,300,180,-,60]
L5-B35-179	[300,60,300,180,-,60]
L5-B35-180	[60,60,300,180,-,60]
L5-B35-181	[180,180,60,180,-,60]
L5-B35-182	[300,180,60,180,-,60]
L5-B35-183	[60,180,60,180,-,60]
L5-B35-184	[180,300,60,180,-,60]
L5-B35-185	[300,300,60,180,-,60]
L5-B35-186	[60,300,60,180,-,60]
L5-B35-187	[180,60,60,180,-,60]
L5-B35-188	[300,60,60,180,-,60]
L5-B35-189	[60,60,60,180,-,60]
L5-B35-190	[180,180,180,300,-,60]
L5-B35-191	[300,180,180,300,-,60]
L5-B35-192	[60,180,180,300,-,60]
L5-B35-193	[180,300,180,300,-,60]
L5-B35-194	[300,300,180,300,-,60]
L5-B35-195	[60,300,180,300,-,60]
L5-B35-196	[180,60,180,300,-,60]
L5-B35-197	[300,60,180,300,-,60]
L5-B35-198	[60,60,180,300,-,60]
L5-B35-199	[180,180,300,300,-,60]
L5-B35-200	[300,180,300,300,-,60]
L5-B35-201	[60,180,300,300,-,60]
L5-B35-202	[180,300,300,300,-,60]
L5-B35-203	[300,300,300,300,-,60]
L5-B35-204	[60,300,300,300,-,60]
L5-B35-205	[180,60,300,300,-,60]
L5-B35-206	[300,60,300,300,-,60]
L5-B35-207	[60,60,300,300,-,60]
L5-B35-208	[180,180,60,300,-,60]
L5-B35-209	[300,180,60,300,-,60]
L5-B35-210	[60,180,60,300,-,60]
L5-B35-211	[180,300,60,300,-,60]
L5-B35-212	[300,300,60,300,-,60]
L5-B35-213	[60,300,60,300,-,60]
L5-B35-214	[180,60,60,300,-,60]
L5-B35-215	[300,60,60,300,-,60]
L5-B35-216	[60,60,60,300,-,60]
L5-B35-217	[180,180,180,60,-,60]
L5-B35-218	[300,180,180,60,-,60]
L5-B35-219	[60,180,180,60,-,60]
L5-B35-220	[180,300,180,60,-,60]
L5-B35-221	[300,300,180,60,-,60]
L5-B35-222	[60,300,180,60,-,60]
L5-B35-223	[180,60,180,60,-,60]
L5-B35-224	[300,60,180,60,-,60]
L5-B35-225	[60,60,180,60,-,60]
L5-B35-226	[180,180,300,60,-,60]
L5-B35-227	[300,180,300,60,-,60]
L5-B35-228	[60,180,300,60,-,60]

Code	Dihedral angles ( $^{\circ}$ ) of M-A-B-C units
L5-B35-229	[180,300,300,60,-,60]
L5-B35-230	[300,300,300,60,-,60]
L5-B35-231	[60,300,300,60,-,60]
L5-B35-232	[180,60,300,60,-,60]
L5-B35-233	[300,60,300,60,-,60]
L5-B35-234	[60,60,300,60,-,60]
L5-B35-235	[180,180,60,60,-,60]
L5-B35-236	[300,180,60,60,-,60]
L5-B35-237	[60,180,60,60,-,60]
L5-B35-238	[180,300,60,60,-,60]
L5-B35-239	[300,300,60,60,-,60]
L5-B35-240	[60,300,60,60,-,60]
L5-B35-241	[180,60,60,60,-,60]
L5-B35-242	[300,60,60,60,-,60]
L5-B35-243	[60,60,60,60,-,60]