

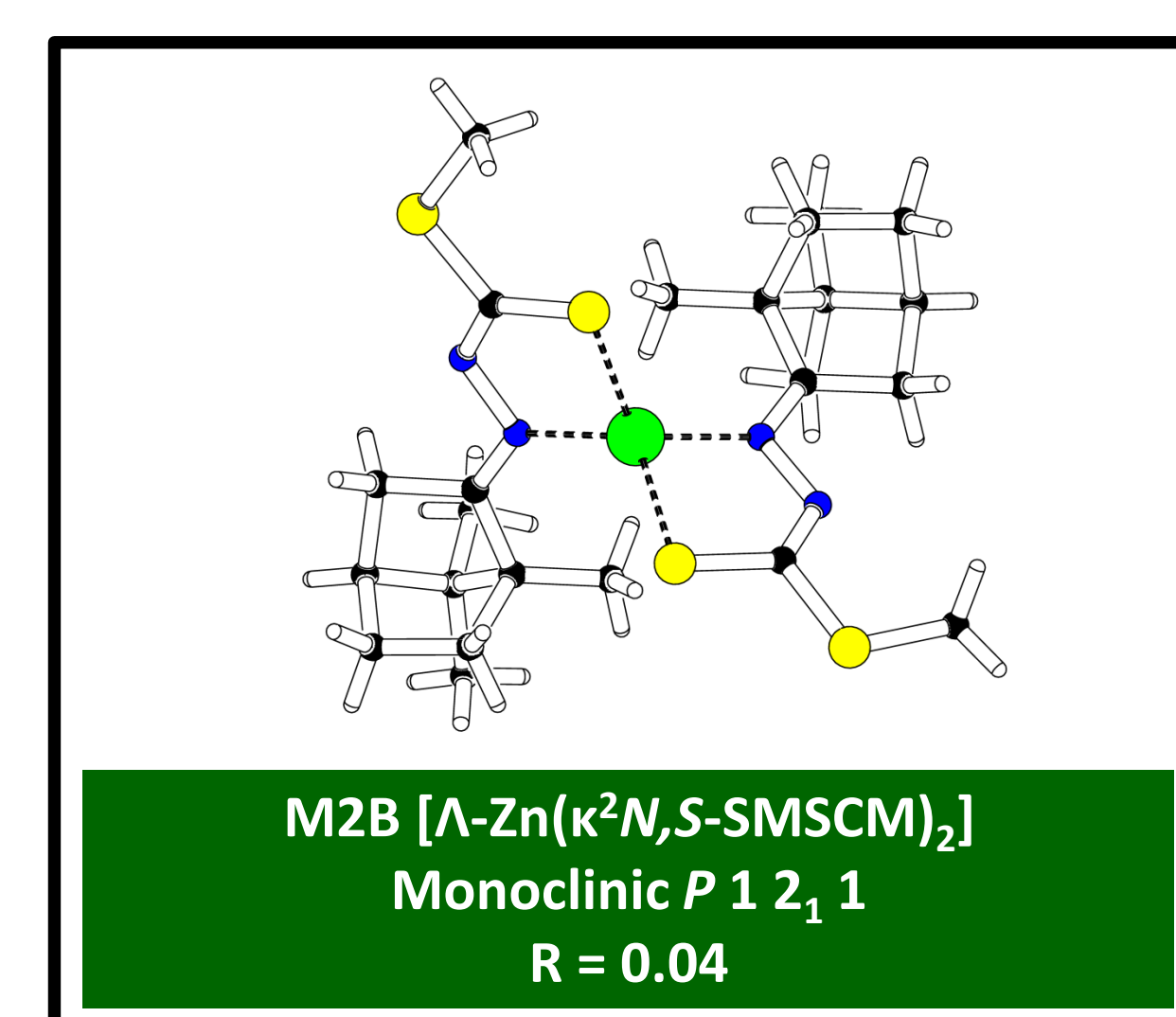
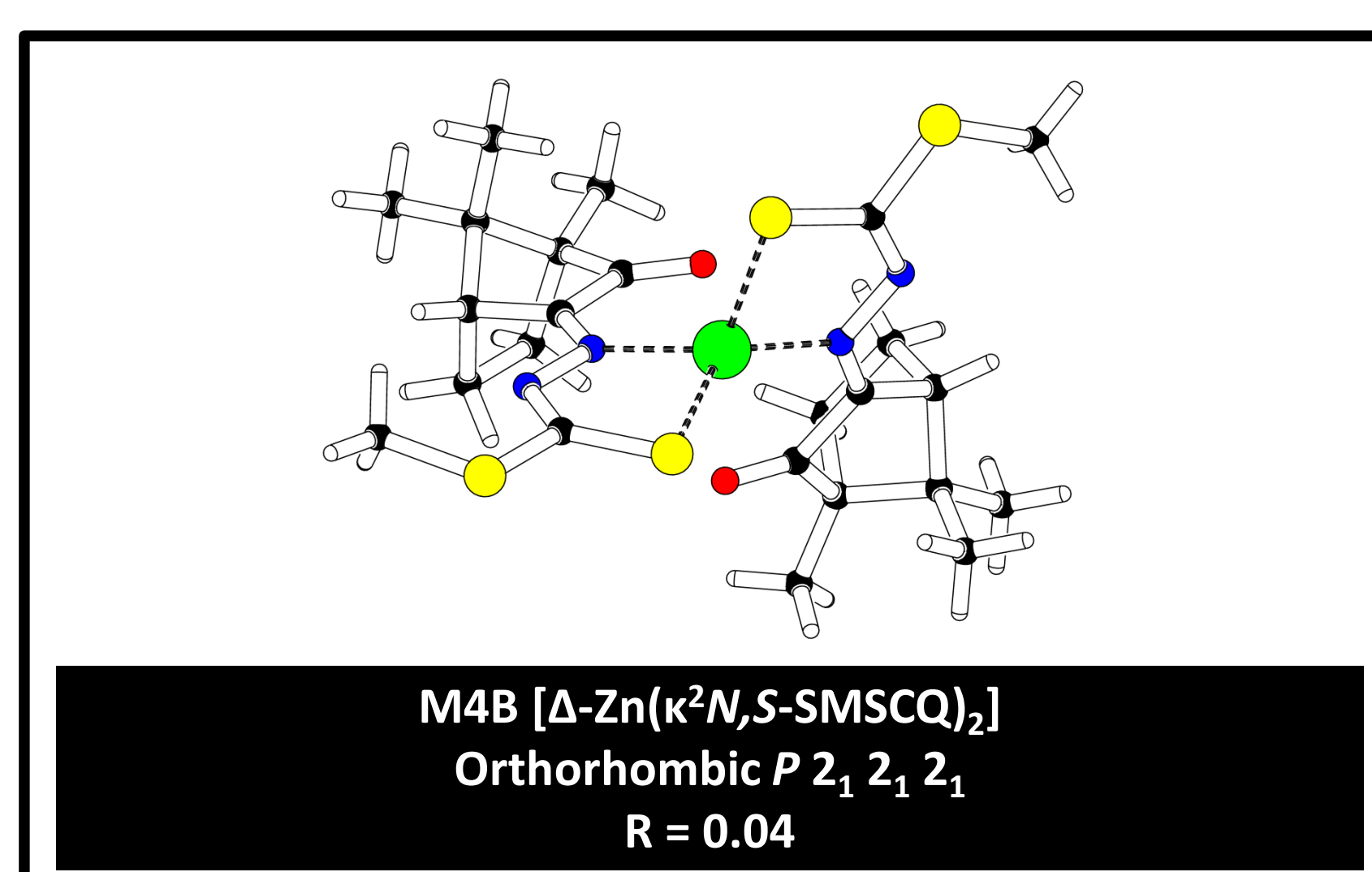
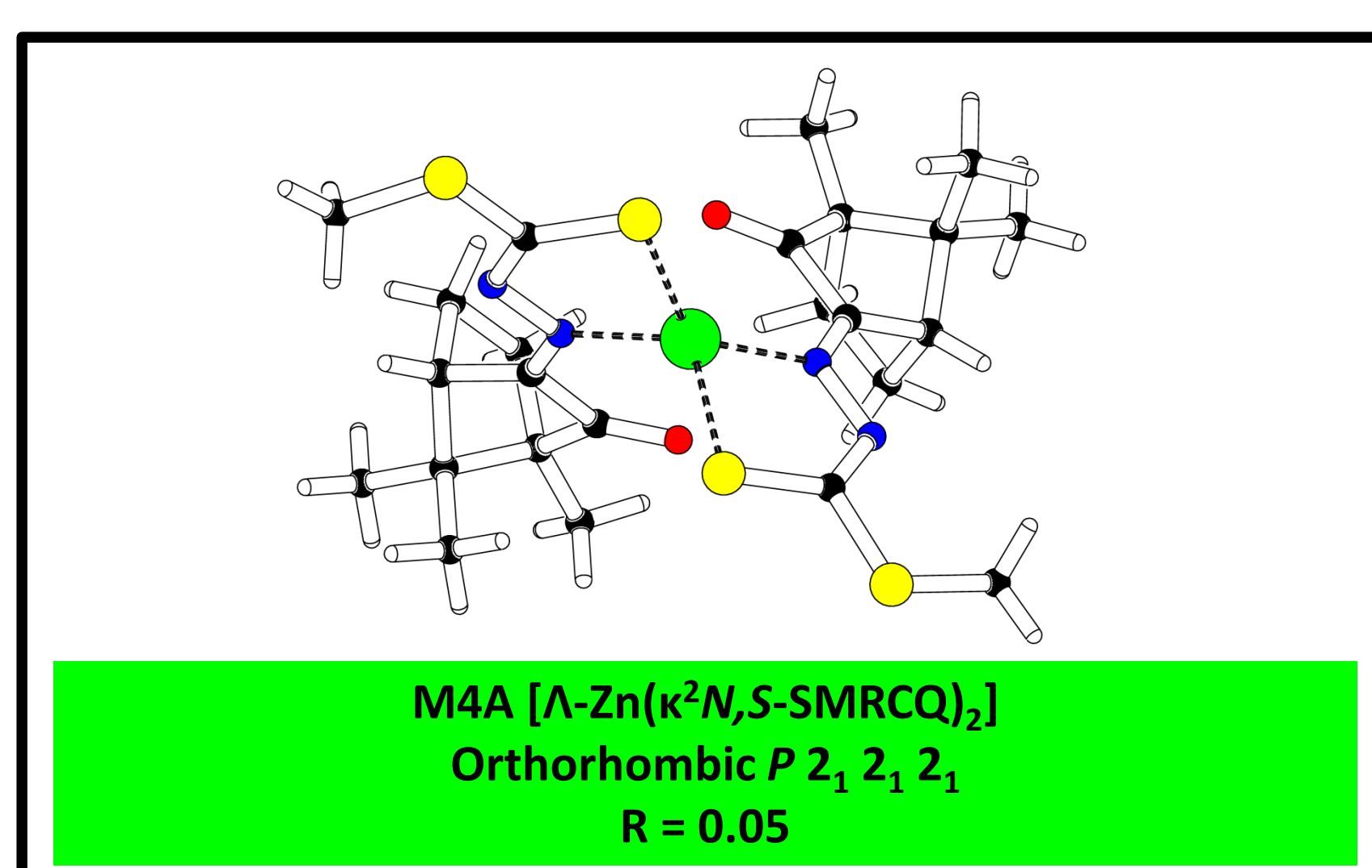
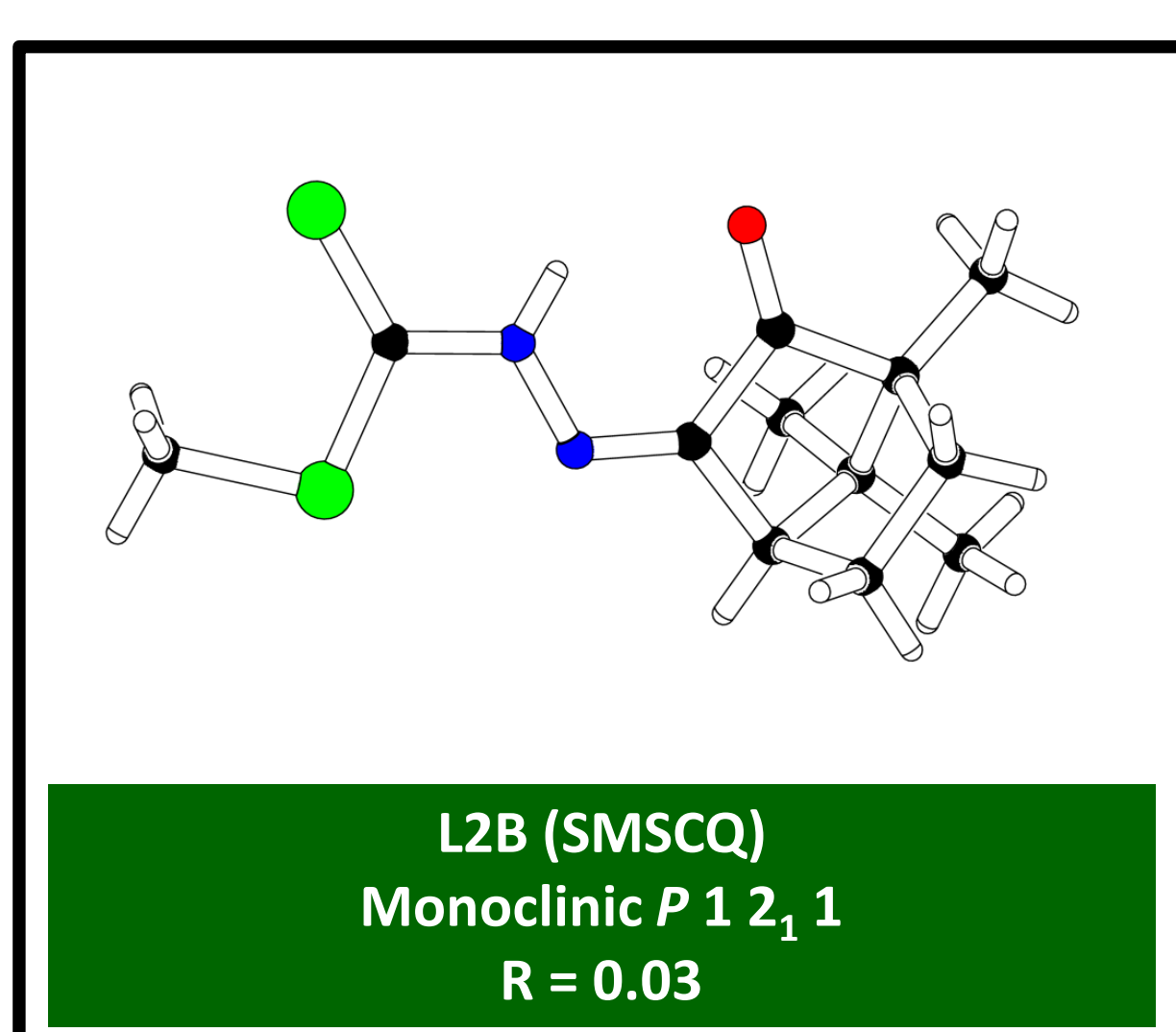
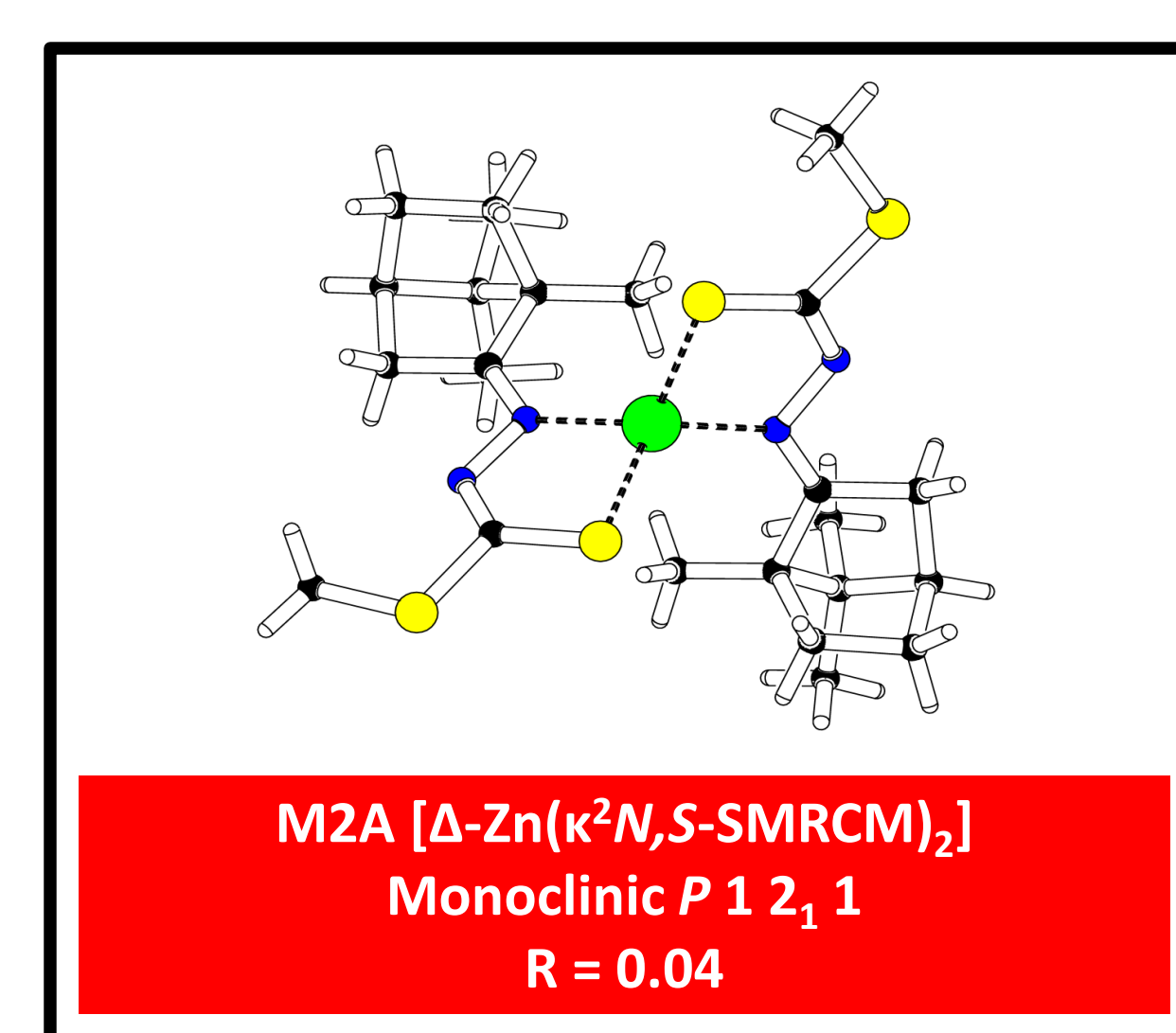
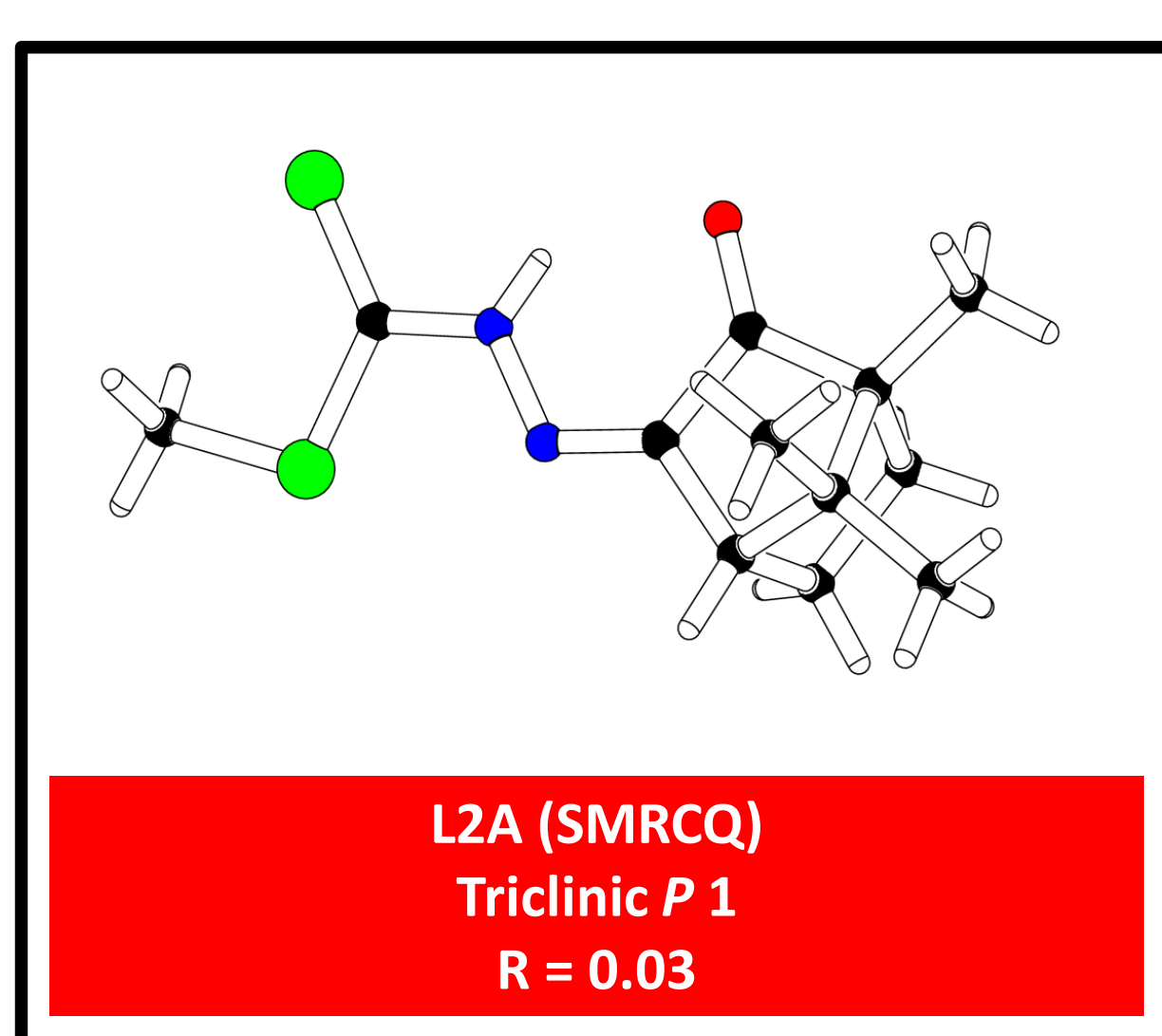
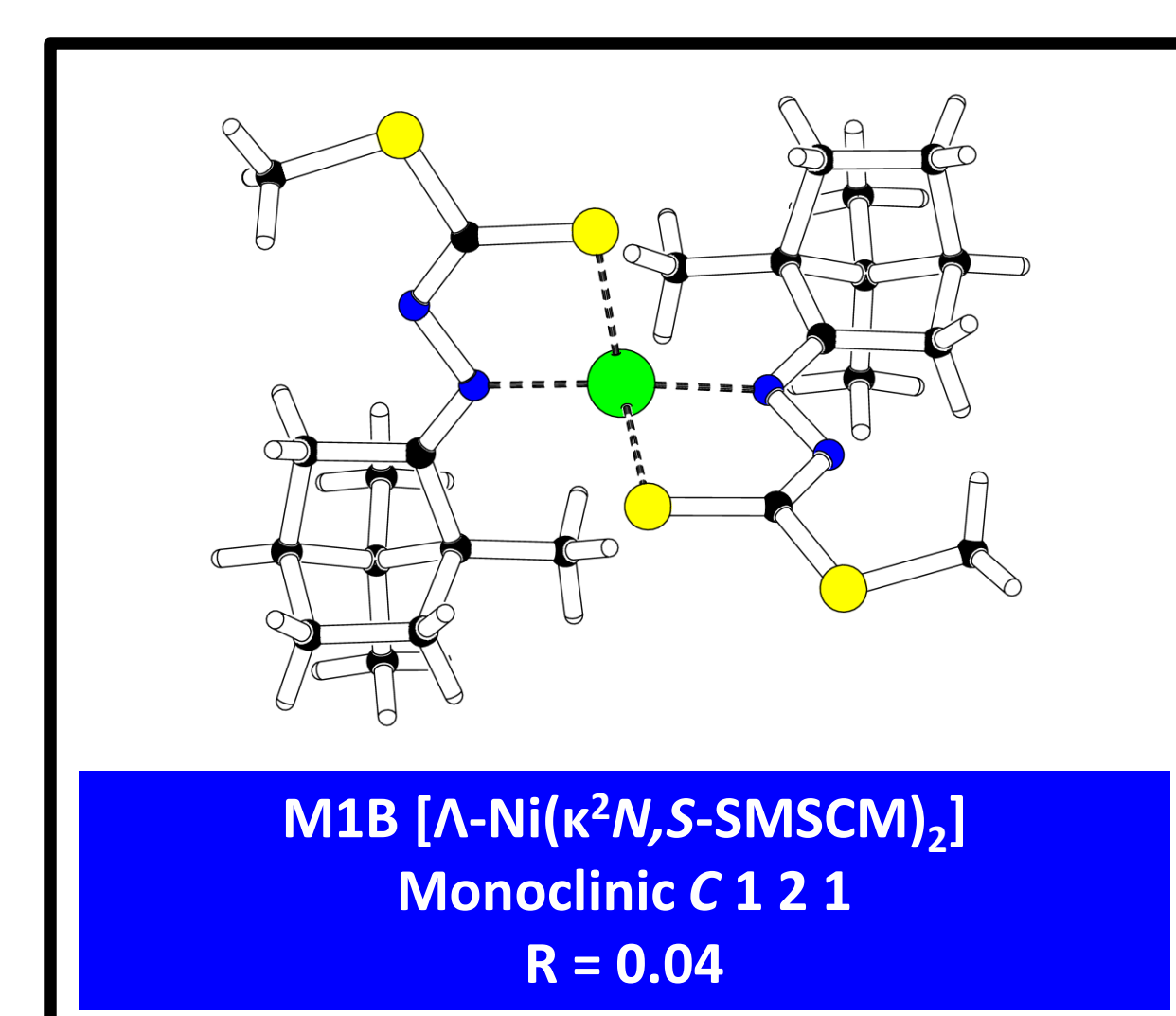
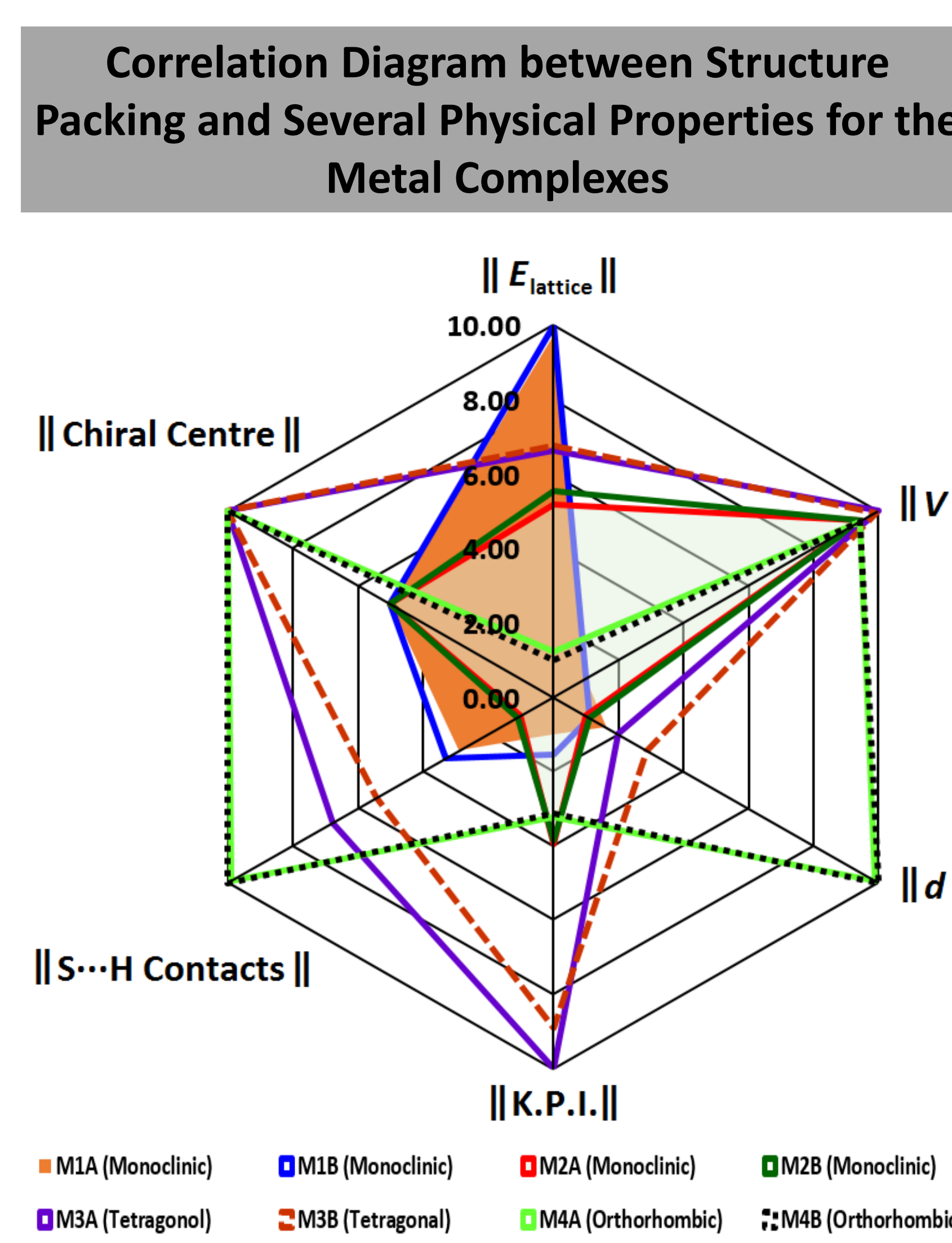
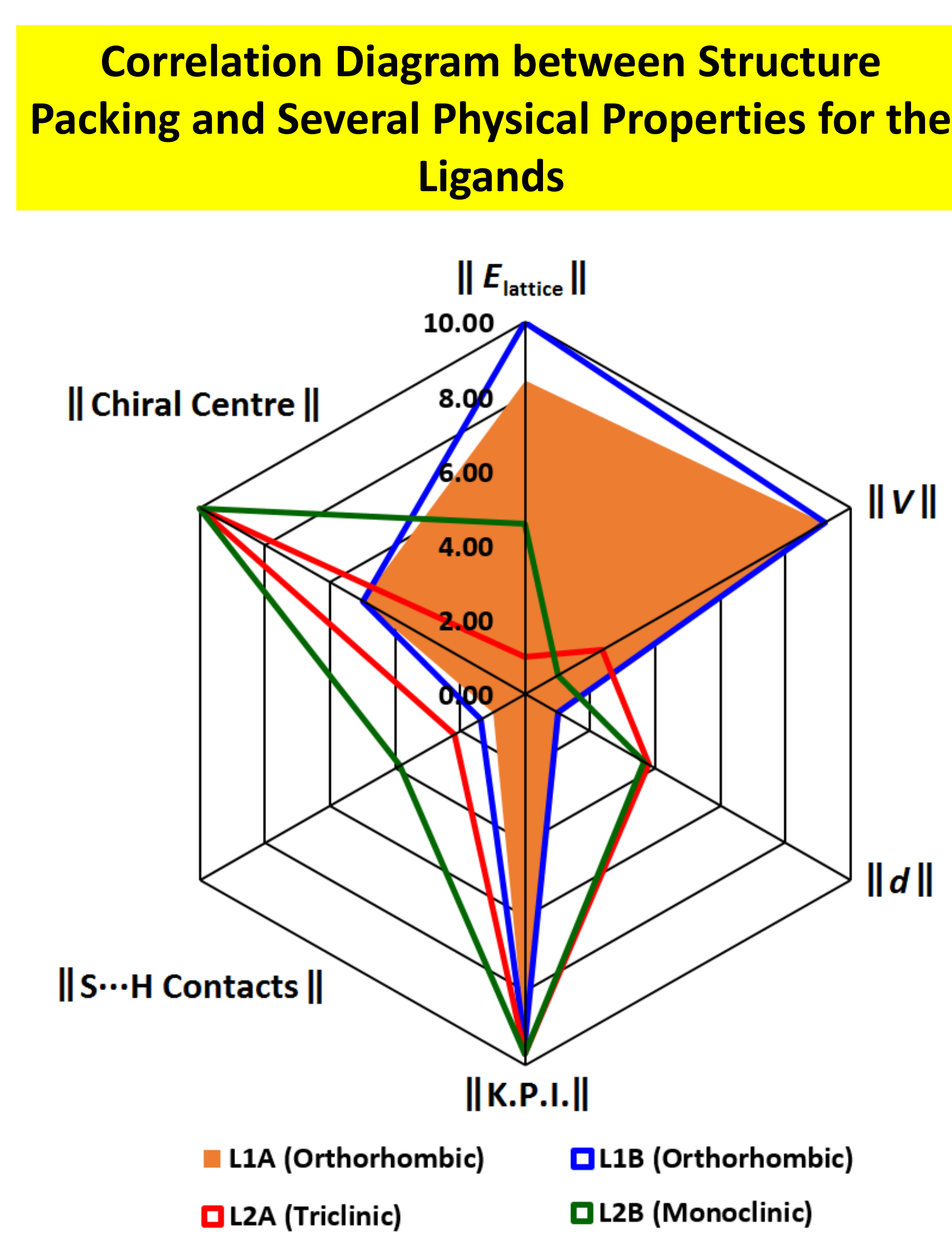
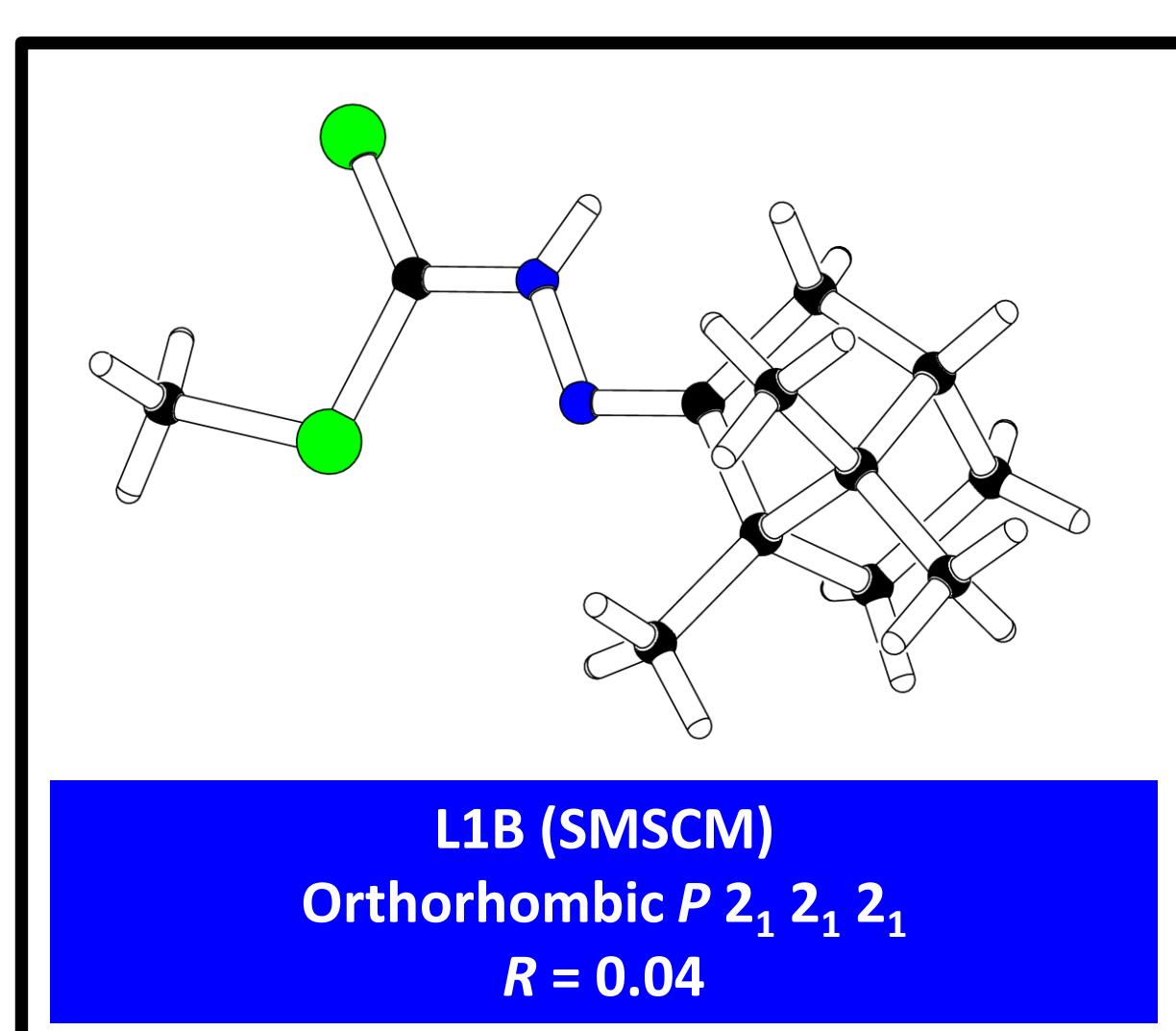
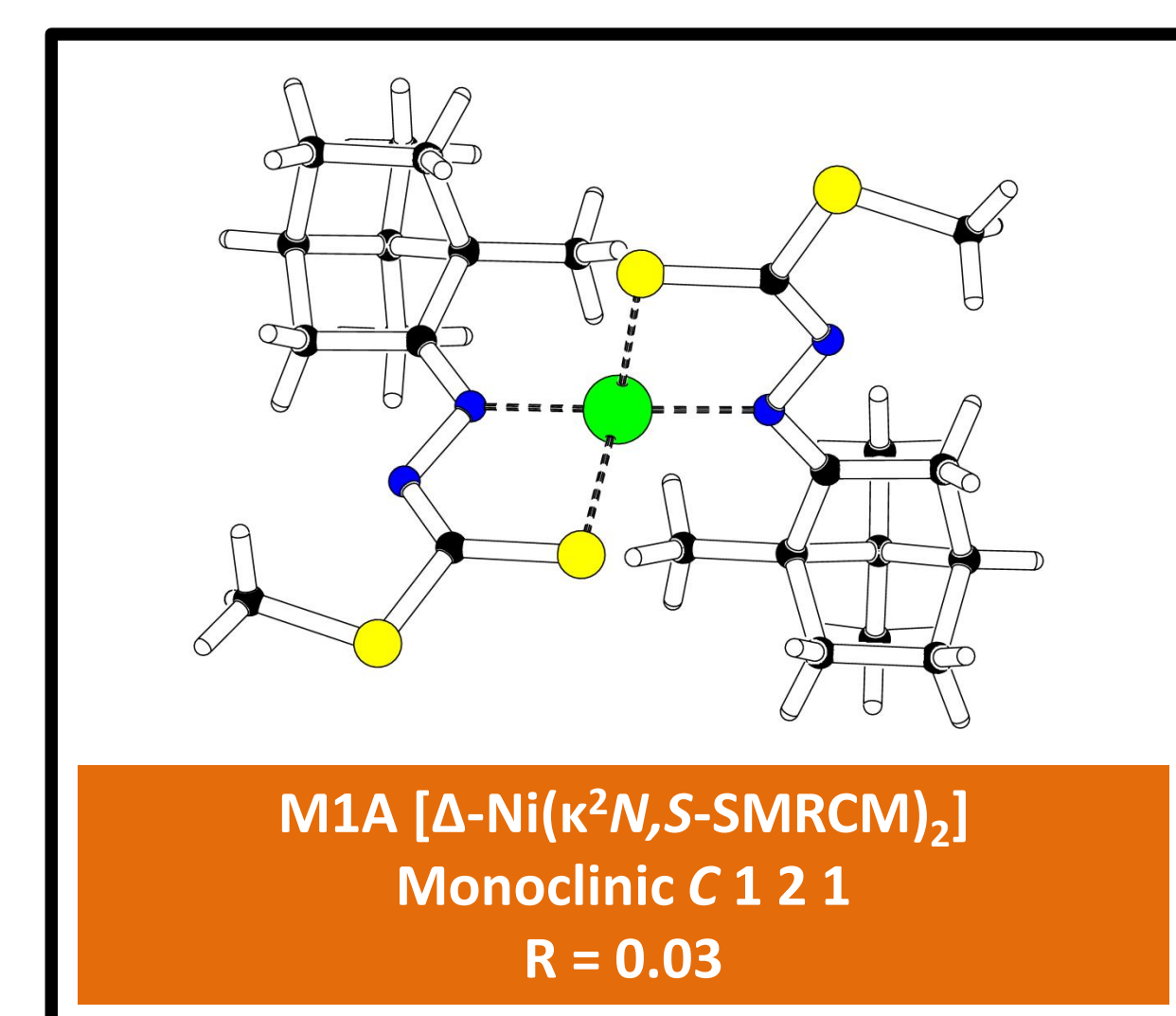
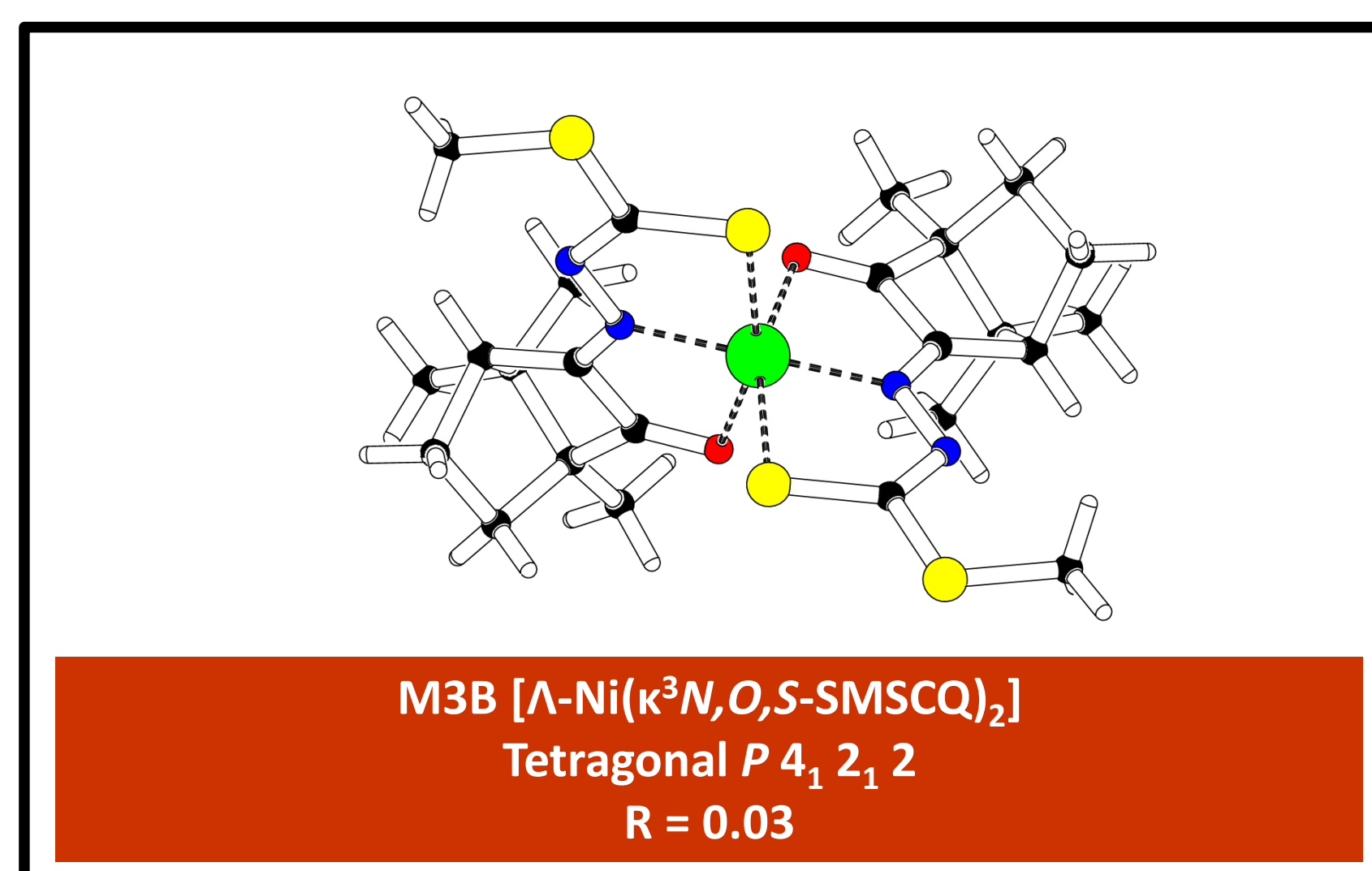
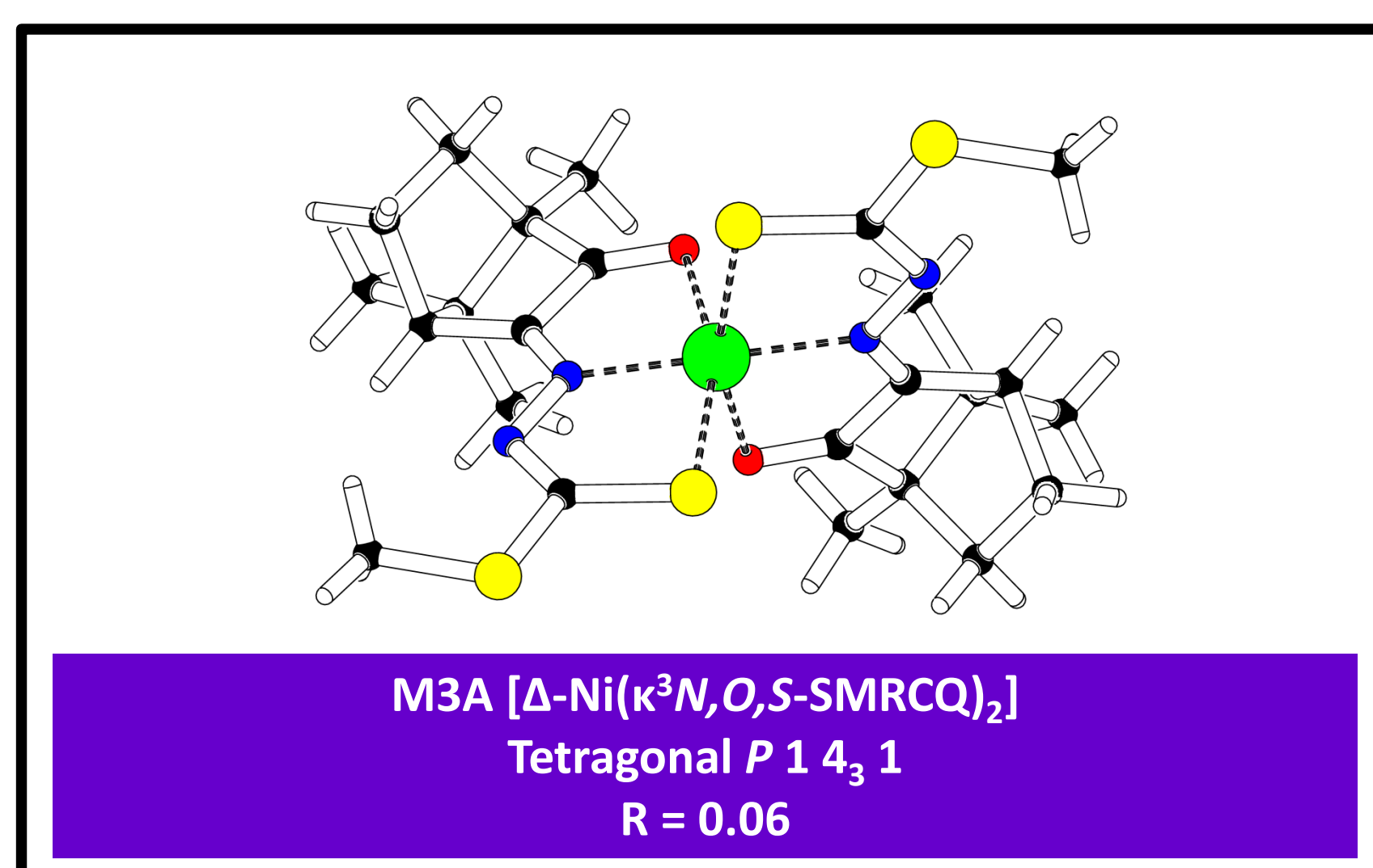
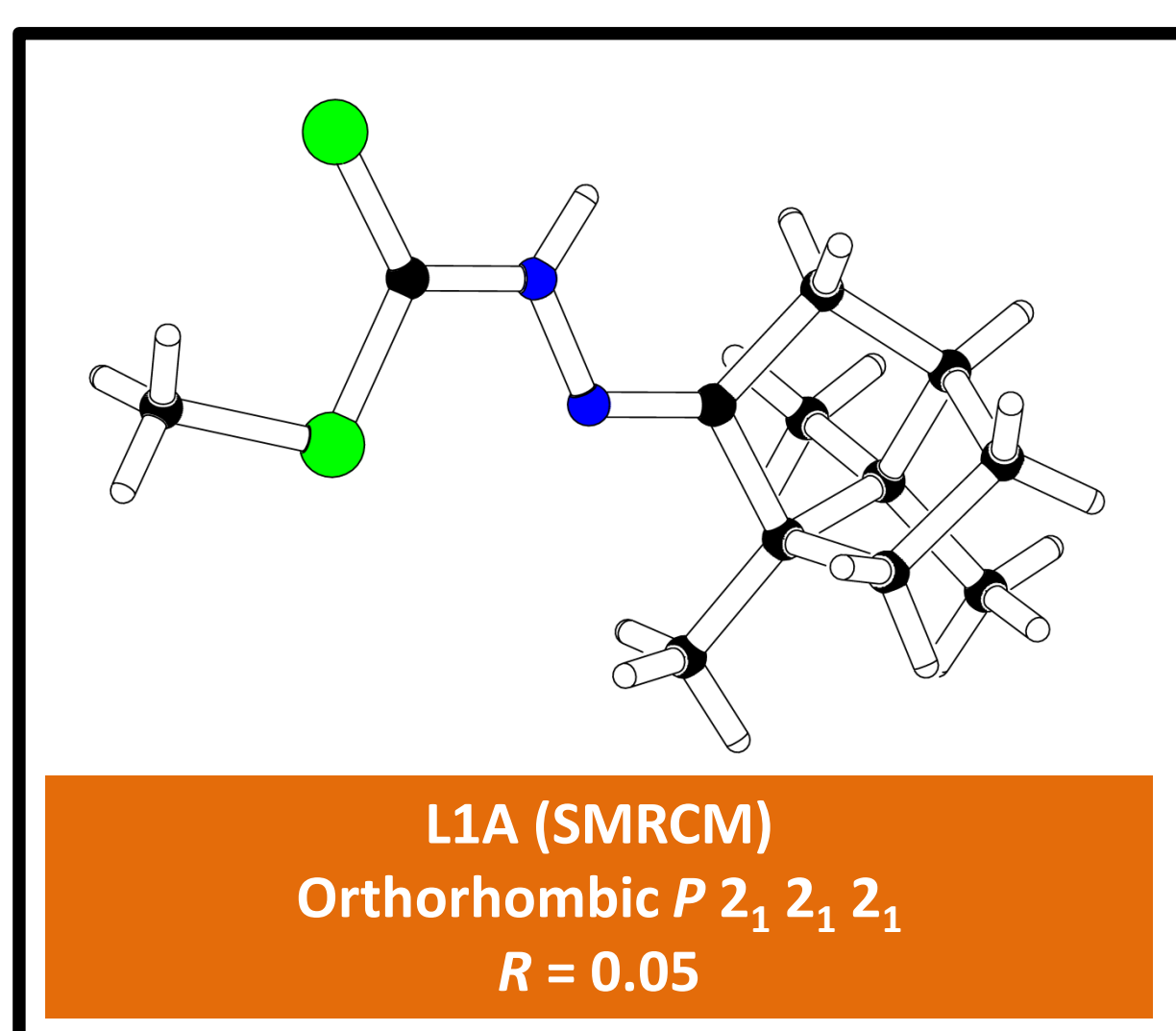
OF STRUCTURAL DIVERSITY AND CRYSTAL PACKING: A CASE STUDY

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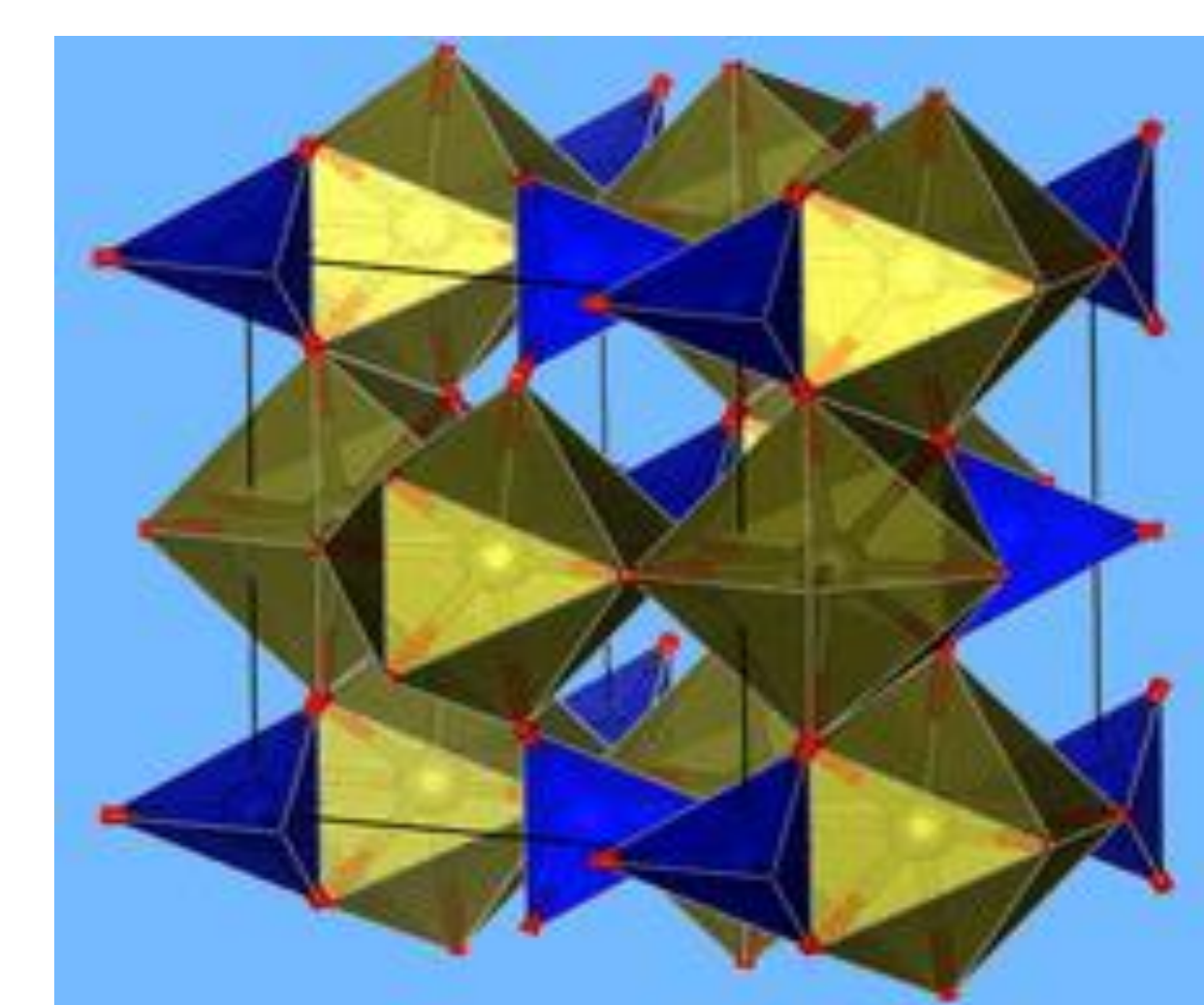
What factors determine crystal packing?



Code	Chiral Centre	Z	Total E_{lattice} (kJ mol ⁻¹)	Cell Volume (Å ³)	Density (g cm ⁻¹)	Molecular Volume (Å ³)	Area (Å ²)	K.P.I. (%)	Relative Composition of Contacts			
									H...H (%)	S...H (%)	N...H (%)	Other (%)
L1A	1R,4R	8	-118.4	2715.42	1.254	332.84	296.24	67.1	57.2	21.0	5.8	3.0
L1B	1S,4S	8	-115.8	2720.00	1.252	333.41	296.47	67.1	58.5	21.3	5.9	3.0
L2A	1R,4S	3	-130.6	1031.22	1.306	337.10	303.64	67.2	55.3	22.0	7.1	15.7
L2B	1S,4R	2	-124.7	689.14	1.303	337.73	303.93	67.2	53.8	23.4	7.7	15.0
M1A	1R,4R	2	-205.6	1391.69	1.359	686.88	509.40	65.9	61.9	25.6	4.9	3.4
M1B	1S,4S	2	-201.0	1395.81	1.355	688.89	510.06	65.9	61.9	25.4	4.9	3.5
M2A	1R,4R	4	-278.6	2825.73	1.354	697.57	506.42	66.2	56.8	27.5	4.6	3.1
M2B	1S,4S	4	-273.0	2824.40	1.355	697.23	506.57	66.3	56.7	27.6	4.6	3.1
M3A	1R,4S	4	-255.4	2914.19	1.362	719.28	515.49	64.3	58.7	28.6	3.9	8.8
M3B	1S,4R	4	-253.3	2898.35	1.369	715.35	513.36	64.3	58.3	28.6	4.1	9.0
M4A	1R,4S	4	-342.9	2815.47	1.425	694.92	520.38	67.3	57.8	26.4	3.7	12.0
M4B	1S,4R	4	-346.2	2814.19	1.426	694.59	520.57	67.3	57.8	26.5	3.7	12.1

Summary

- For ligands, their crystal packing is found to be determined by the relative composition of contacts, density as well as number of stereogenic centre. The E_{lattice} for crystal system is in the order of orthorhombic < monoclinic < triclinic.
- For metal complexes, the crystal packing is influenced by the relative composition of close contacts and density. The E_{lattice} for crystal system is in the order of monoclinic < tetragonal < orthorhombic.
- Overall, it is observed that the **relative composition of close contacts** and **crystal density** are the most influential factors in determining the packing of a crystal system. Greater cell density and relative composition of close contacts generally lead to greater lattice energy.



Understanding of packing behaviour may help in successful crystal structure prediction!

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