

TABLE I. Composition of the active space with 76 orbitals for FeMoco.

group	orbital	orbital index
left cubane		
1	left end	1, 2
2	Fe1 3d	3, 4, 5, 6, 7
3	S 3p	8, 9, 10, 11, 12, 13, 14, 15, 16
4	Fe2 3d	17, 18, 19, 20, 21
5	Fe3 3d	22, 23, 24, 25, 26
6	Fe4 3d	27, 28, 29, 30, 31
central part		
7	S 3p, C 2s2p	32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44
right cubane		
8	Fe5 3d	45, 46, 47, 48, 49
9	Fe6 3d	50, 51, 52, 53, 54
10	Fe7 3d	55, 56, 57, 58, 59
11	S 3p	60, 61, 62, 63, 64, 65, 66, 67, 68
12	Mo8 4d	69, 70, 71, 72, 73
13	right end	74, 75, 76

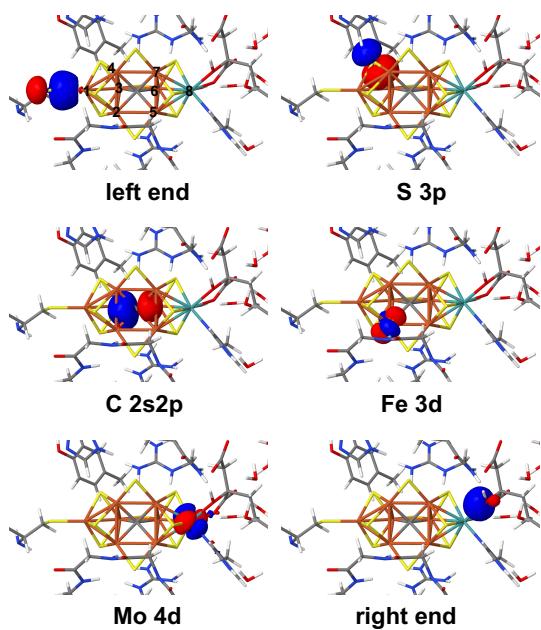


FIG. 3. Illustration of some selected active orbitals for FeMoco in the active space model CAS(113e,76o) constructed in this work.

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