

The “edited\_XXII...” cifs have the same geometry as those originally submitted in the blind test but have been corrected to remove distortions that resulted from imposing symmetry with pymatgen.

The cif file “PBE0\_MBD\_Marom.cif” (and the corresponding edited file “edited\_PBE0\_MBD\_Marom.cif”) is an extra set of structures calculated with PBE0+MBD. These were not submitted in the blind test but are included here for reference.

Anthony Reilly, June 2016