Results and Discussion

The included GAMS data file corresponds to $C_{50}H_{66}O_6 \bullet C_3H_7NO$, which has 61 atoms in the asymmetric unit and is Structure 8 in Chapter 4 of [4]. The MINLP model M1 possesses 23,424 binary variables out of a total of 23,530 variables. There is a total of 551 constraints, all of which are linear. The only nonlinearities arise in the objective. As of the time of this writing, M1 remains unsolved with all solvers tried (BARON 8.1.5, SBB, DICOPT, alphaECP 1.63, LINDOGLOBAL) within a time limit of three CPU hours. Feasible solutions were obtained by BARON, DICOPT, and alphaECP, with corresponding objective function values equal to 0.2293, 0.2752, and 0.4743. When BARON was run with the probing option turned off, a feasible solution with an objective function value equal to 0.1164 was reported but the lower bound provided was still 0.

The MIP model M2 involves 23,529 binary variables, a total of 24,055 variables, and 1181 constraints. Running CPLEX on M2 with $U = 2 \max_k s_k$ for three CPU hours gave an upper bound of 0.0797, with a lower bound of 0. Running CPLEX on M2 with $U = 0.08 + \max_k s_k$ for three CPU hours gave an upper bound of 0.0957, with a lower bound of 0 once again.

The MIP model M3 involves 23,529 binary variables out of a total of 23,740 variables. There are 761 constraints present. Running CPLEX on M3 for three CPU hours gave an upper bound of 0.0823, with a lower bound of 0, as was the case with all previous models.

Concluding remarks

Models M1, M2, and M3 are applicable only to centrosymmetric space groups. Variants and generalizations of the above formulations, including formulations for non-centrosymmetric space groups, smooth formulations based on a 2-norm figure of merit, and equivalent mixed-integer linear programming formulations, are presented in [4].

None of the solvers tried thus far has managed to prove global optimality for the above models. Despite the fact that all solvers returned very different objective function values and solution points, all solutions provided correspond to a physically meaningful structure, with a mean phase error well below 5% for the test problem solved. For centrosymmetric structures, like the one solved here, this happens because it is not the actual value of the calculated structure factors, E_m, that matters but their signs alone determine the crystal structure.