Oral presentation

What I gained from Erice

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The first Erice School on Advanced Studies of Direct Methods in Crystallography remains a milestone. Already I had a background in structural determinations developed during my thesis and post-doc stages in USA (UW and NW). At that time, the task was not so easy even if some metal atom allowed a fruitful usage of the Patterson methods. On the other hand, the discovery of Direct Methods (DM) was a breakthrough in the phase determination problem for most X rayed crystals (proteins had still to wait). The 1952 Sayre's Equation had shown how a structure factor may be derived from pairs of other known ones and this originated a worldwide fervour for the development of mathematical/probabilistic methods. Hence, the crystallographic community considered the time ripe for illustrating the DM foundations and the Ettore Majorana Centre (established by A. Zichichi in Erice) was chosen as the seat of an advanced School, later become a permanent one. The person who led the operation was Ludovico Riva di Sanseverino (professor in Bologna but with a genuine Sicilian origin [1]), who organized a memorable event in which borderline science alternated with entertainment activities, often embellished by his choirs. Mike Woolfson (University of York), already an excellence in the DM field as the scientific Director of the School summoned some of the leading experts as teachers. Amongst them, the Italian pioneer, Giuseppe Allegra, opened the sessions. Another impressive character was David Sayre himself (1924-2012), not only for having produced the DM seminal idea, but also for the friendly behaviour and the provocative stories, that he told us during meals and free time. Later in the career, Sayre confirmed to be a giant in crystallography also for showing that the crystallinity (periodicity) of the sample is not essential for a structure determination. This was possible by opportunely focusing X-rays on a small portion of the specimen (e.g., a single biological cell). As the Chair of the XX IUCr Congress in Florence (2005), I had the honour of having Dr. Sayre as a Plenary Lecturer, who reported on these extraordinary findings. Moreover, since I remained a member of the Organizing Committee of the following IUCr Congress (Osaka, 2008), I strongly supported the award of the Ewald Prize to Sayre himself. The other extraordinary star of the Erice School was Herbert Hauptman, who in 1985 became Nobel laureate together with Jerome Karle for their joint DM development. Unfortunately, the latter was not present at the first Erice School, which had clearly forerunning character. Hauptman was accompanied by two young collaborators from his Buffalo lab, namely Bill Duax and Suzanne Fortier, whom I made friend with. Later, Bill, as IUCr President, gave a strong support to our Congress in Florence, whereas Suzanne abandoned crystallography but for many years she was Rector in charge of the prestigious McGill University in Montreal. Amongst other teachers and students, I recall Peter Main (working with Woolfson in York), who developed one of the most efficient computer programs of the time, named MULTAN. Two other Italian participants, such as P.F. Zanazzi (Perugia) and D. Viterbo (Torino), had been working in the Woolfsoon's lab. In particular, Viterbo presented an illuminating lesson on the phase relationships and also acted as tutor in practical sessions to clarify obscure points. My friendship with Davide lasted till his final days in 2017 [2]. Also, some of the French and Dutch leading labs had representatives such as G. Germains, G. Tsoucaris and P. Beurskens. Finally, another outstanding personality, who appeared on the scene, was Carmelo Giacovazzo (Univ. of Bari), who proved to be already a top DM expert. In a still broken English, he intervened in passionate discussions with the most renowned scientists without showing any inferiority complex. In the years to come, Carmelo confirmed his extraordinary competence by introducing innovative theories, which were translated into practical computer programs by researchers from different Italian labs. For many years and still today, the package SIR has helped solving any type of structure worldwide. I suspect that a Nobel prize on DM, not including Carmelo, may have been a little precocious! Finally, the great enthusiasm, which I matured at the School, persisted after returning to my own research interests. While I did not devote all the necessary efforts to deepen DM math underpinnings, their usage was fundamental for my goals. In fact, it extended my capabilities of accumulating structural data in selected areas of chemistry and allowed me to focus mostly on the chemical information contained in structures. I compared a plethora of chemical bonds in different environments and started finding implications for the chemical functionality and reactivity of the compounds. At some point, I had to decide to complement crystallography with other tools such as those of Quantum Mechanics in order to evaluate bond energies and follow their evolution. Again, I had the luck of overlapping with an exceptional QM mentor, namely Roald Hoffmann, who was Nobel Laureate in 1981. Remarkably, the important combination of the two techniques was premonitorily emphasized by Linus Pauling in his 1954 Nobel Lecture. Hence, I see another link with Erice, namely the award of the first Ettore Majorana prize (1989) to L. Pauling.

[1] Mealli, C. (2010). J. Appl. Cryst., 43, 946.

[2] Mealli, C. & Milanesio, M. (2017). Acta Cryst., A73, 375.