The lines-of-force landscape of interactions between molecules in crystals. Cohesive vs. tolerant and "collateral damage" contact

Angelo Gavezzotti

Dipartimento di Chimica Strutturale e Stereochimica Inorganica, Università di Milano,
via Venezian 21, 20133 MIlano, Italy

Correspondence e-mail: angelo.gavezzotti@unimi.it

Supplementary Information

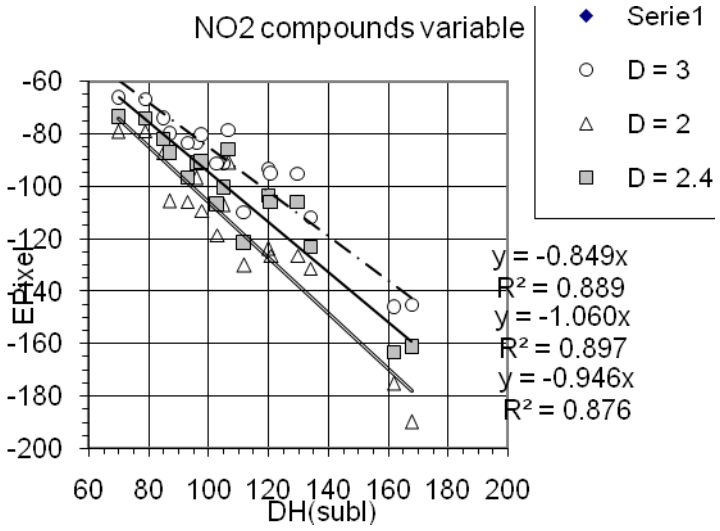


Figure S1. Plot of PIXEL lattice energies versus sublimation enthalpy fore nitro crystals of nitro compounds, for different values of the PIXEL dispersion screening parameter D.

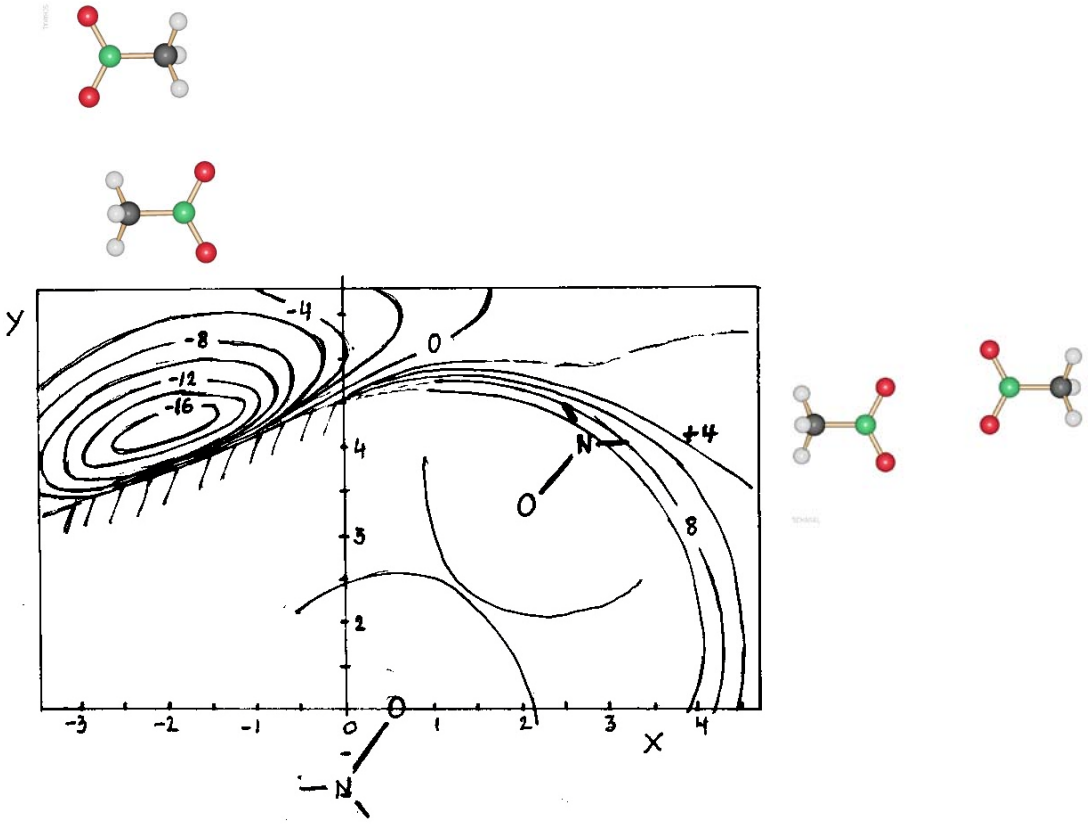


Figure S2. A section of the PIXEL energy map for the approach of two nitromethane molecules. The N atom of one molecule is at $x = y = 0$, and the map shows the energy for a coplanar dimer ($z = 0$) with the N atom of the second molecule at x, y and C-N bonds parallel. The rightmost part of the map shows the potential field for an oxygen-oxygen approach with moderate repulsion all the way. The circles show an approximate oxygen radius.

Figure S3. The structure determinants (molecular pairs) in the crystal structure of nitroguanidine (CSD refcode NTRGUA03). Labels are as in Figure 5. Some relevant atom-atom distances are given (Å units).

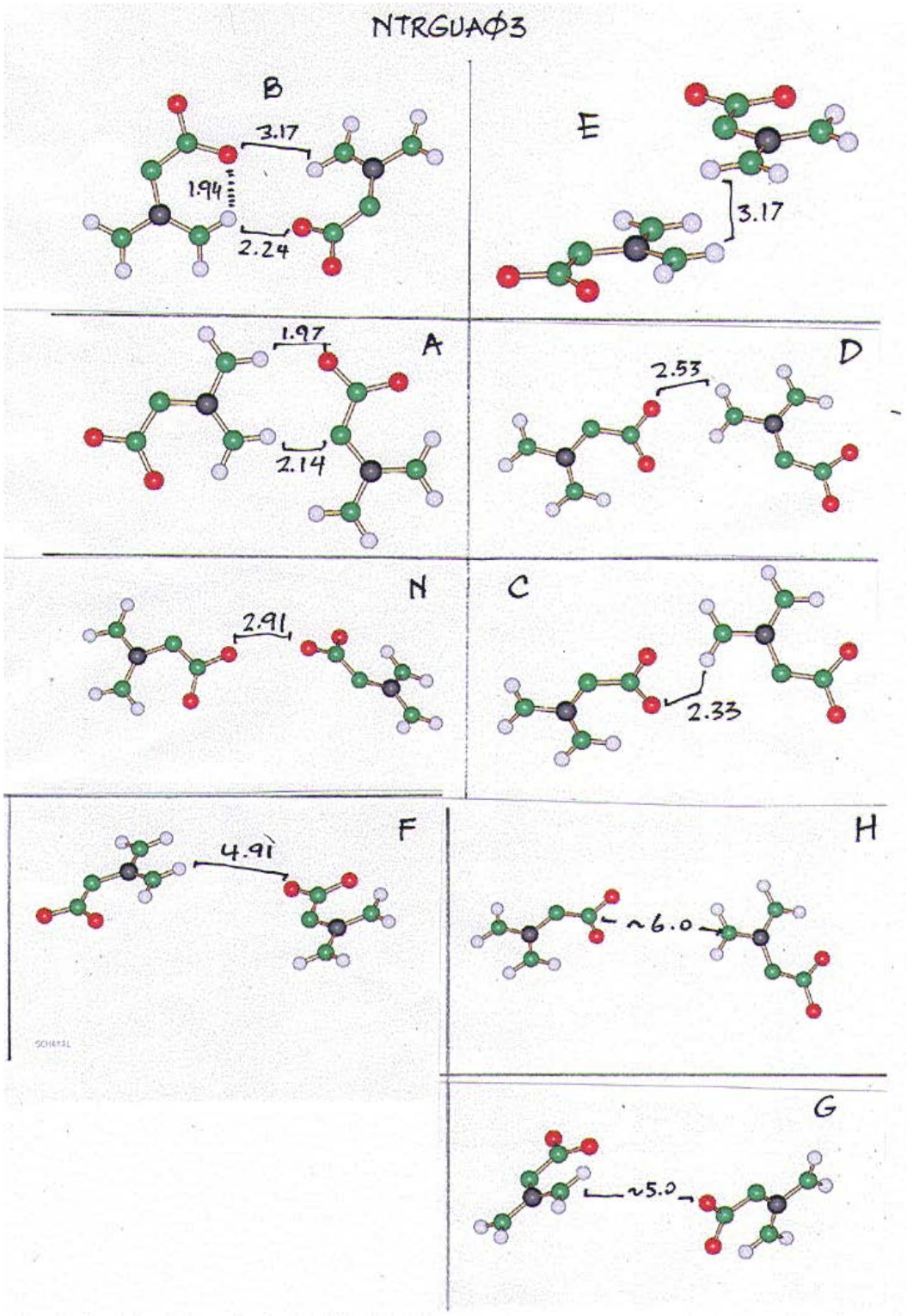


Figure S3 (continued). The structure determinants (molecular pairs) in the crystal structure of nitroguanidine (CSD refcode NTRGUA03). Labels are as in Figure 5. Some relevant atom-atom distances are given (Å units).

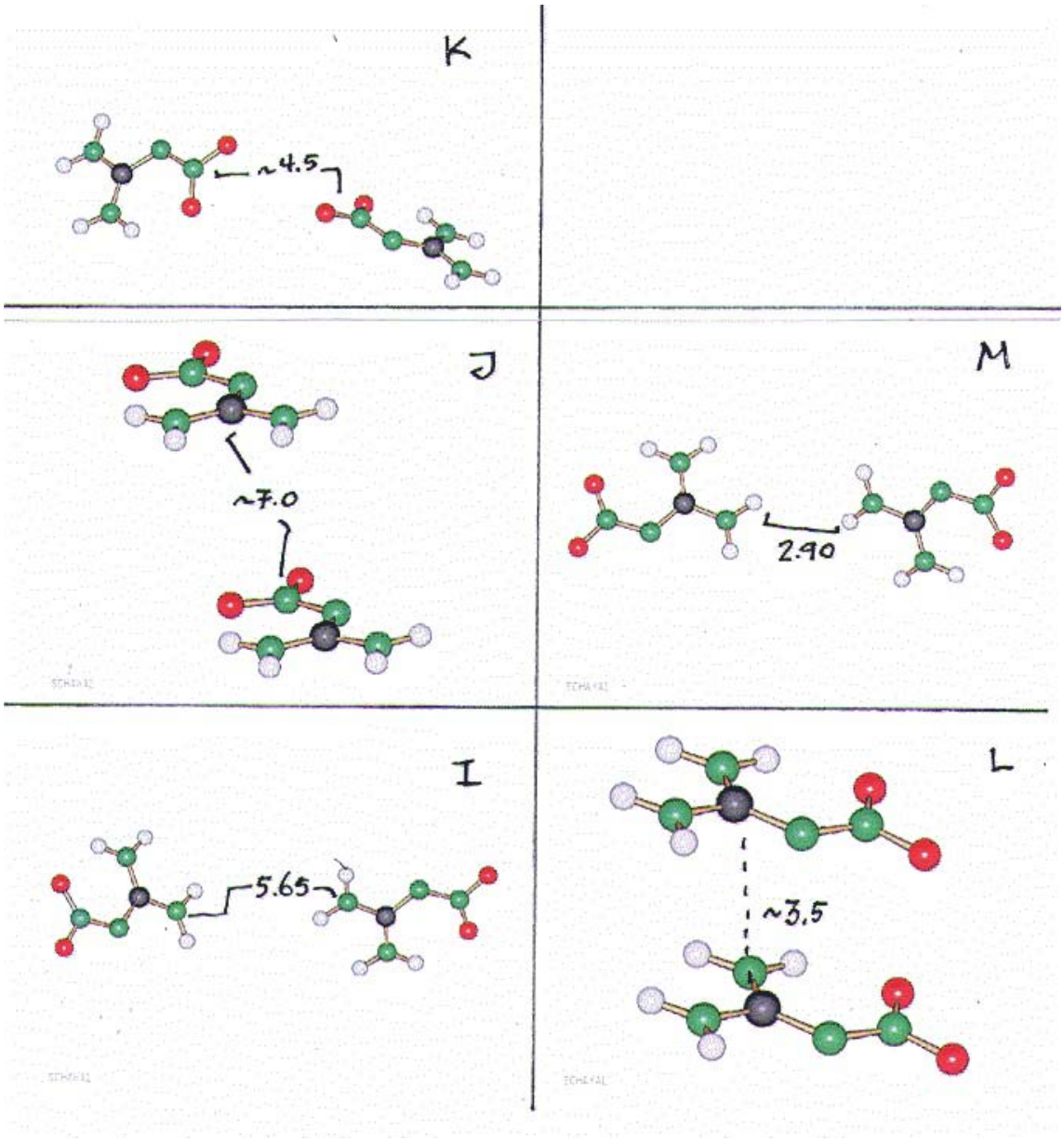
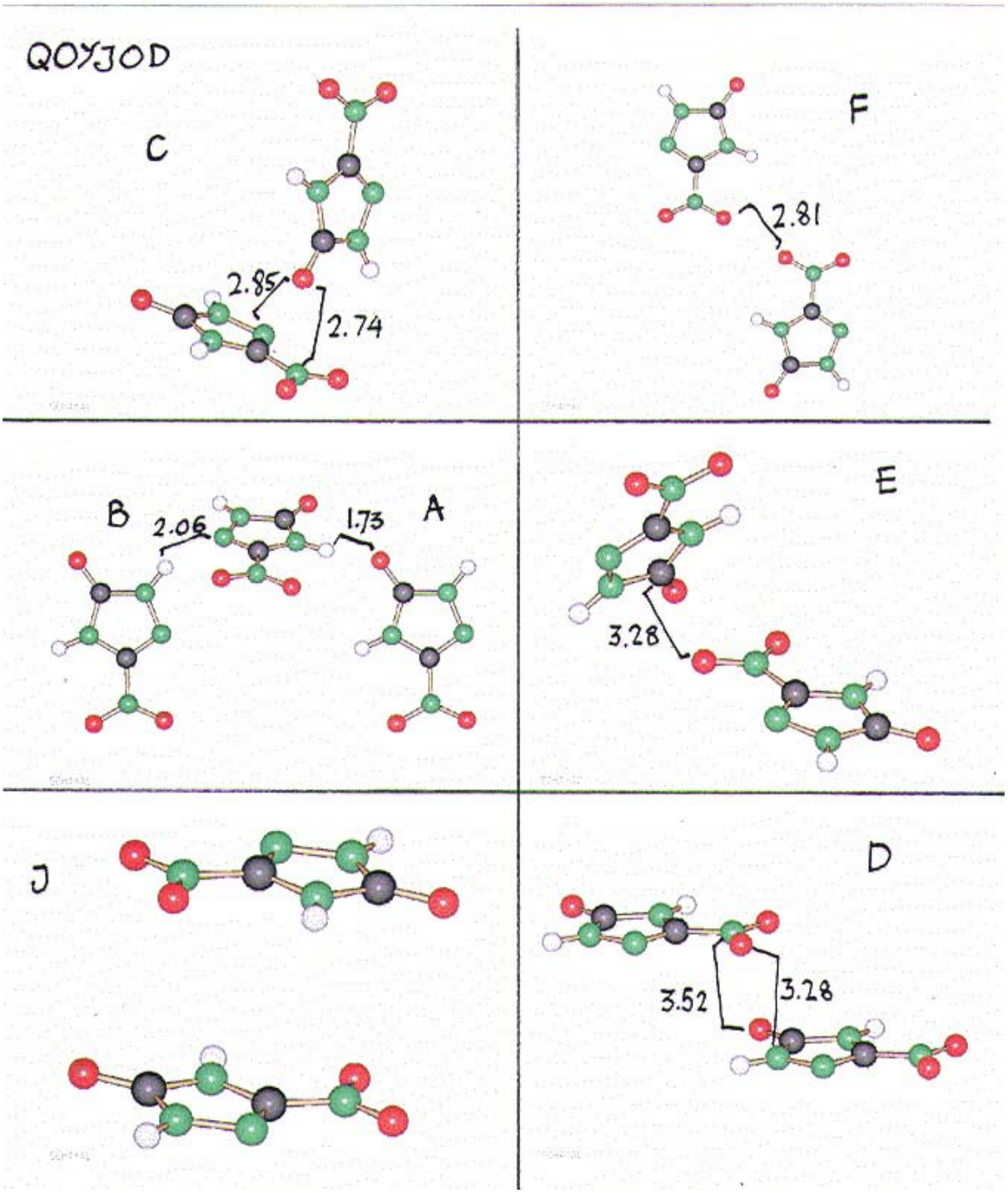


Figure S4. The structure determinants (molecular pairs) in the crystal structure of QOYJOD. Labels are as in Figure 6. Some relevant atom-atom distances are given (Å units).



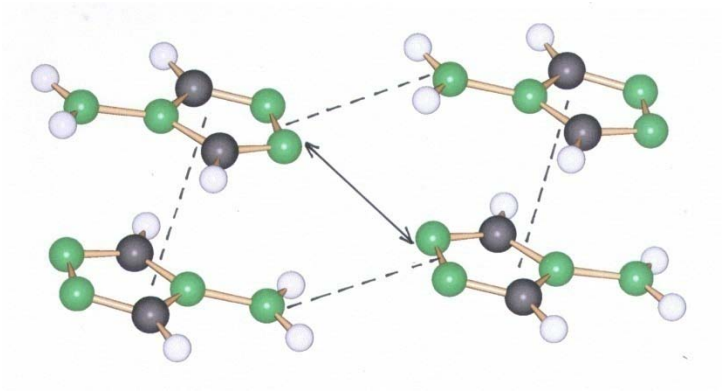


Figure S5. As in Fig.8, but for the crystal structure of 4-amino-1,2,4-triazole, CSD refcode KUTHAI. The NH_2 … N=N interaction and the stacking interaction are moderately stabilizing, the forced N=N … N=N interaction is destabilizing, with N…N distances of 3.90 Å. The two stabilizing contacts (broken lines) are -27 and -25 kJ mol^{-1}, the repulsive interaction (full arrow) is +16 kJ mol^{-1}.

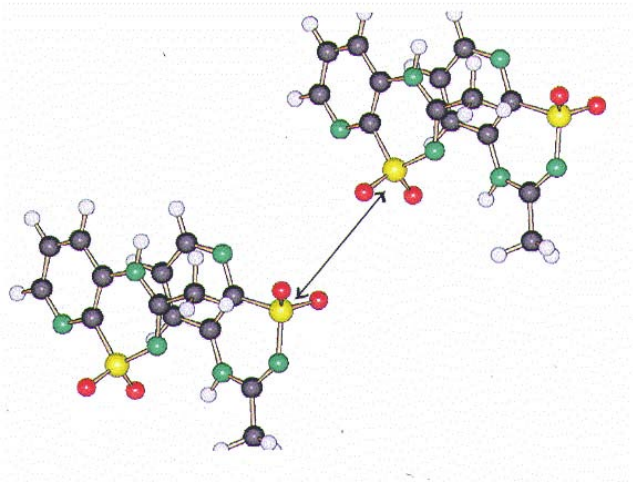


Figure S6. Net repulsive destabilizing interaction between SO2 groups in the crystal structure of YOWXIR. This is the strongest repulsive interaction found in our data set (+20 kJ mol^{-1}).

Figure S7. The structure determinants (molecular pairs) in the crystal structure of DL-alanine (CSD refcode DLALNI01). Labels are as in Figure 13. Some relevant atom-atom distances are given (Å units).