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ELECTRONIC SUPPLEMENTARY INFORMATION

Rigid ferrocene-ferrocene dimer as a common building block in the crystal structures of ferrocene derivatives

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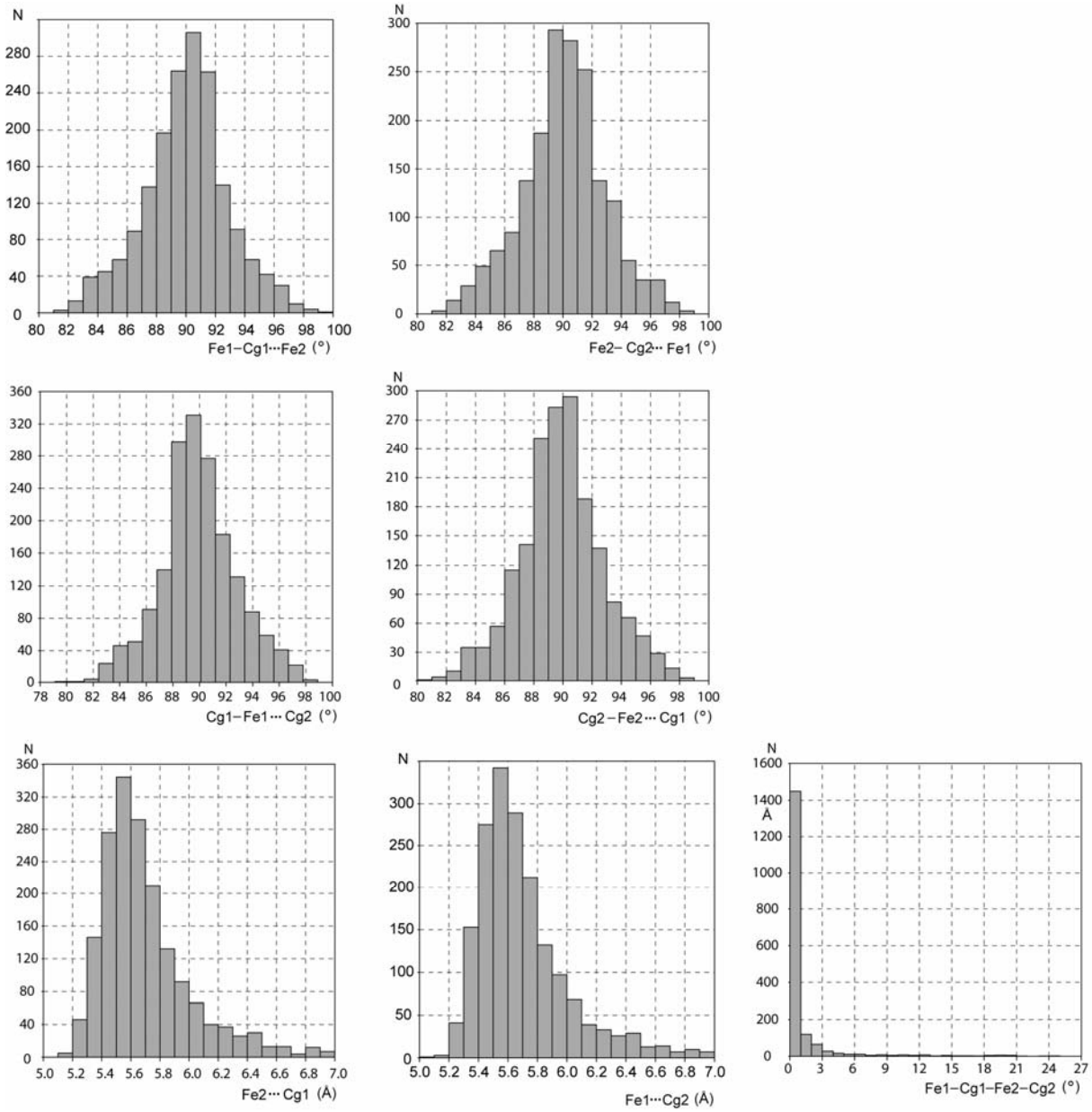


Fig. S1 Distribution of the geometrical parameters describing FcD in crystal structures containing monosubstituted Fc moieties. Cg is a centroid of Cp ring.

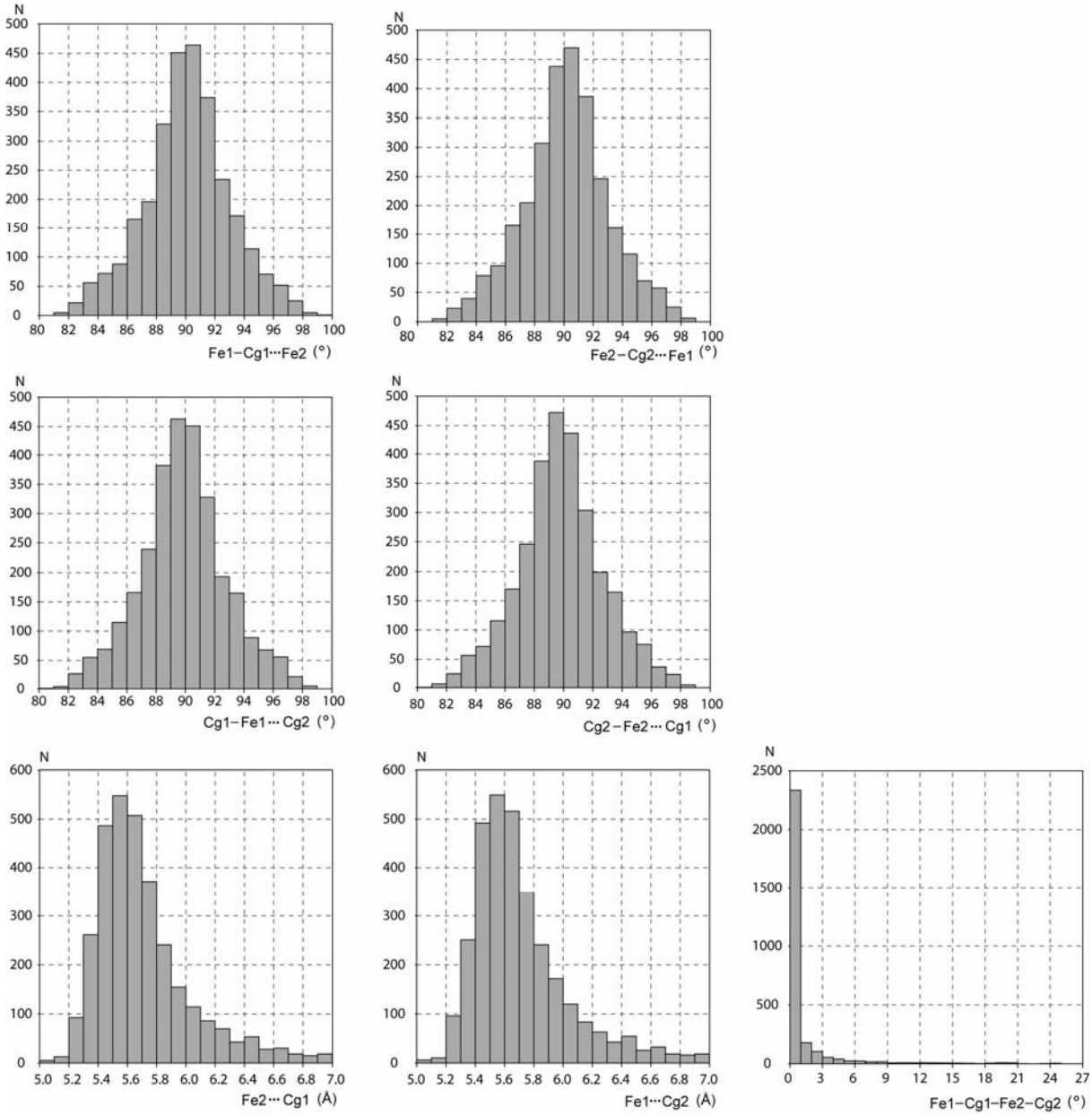
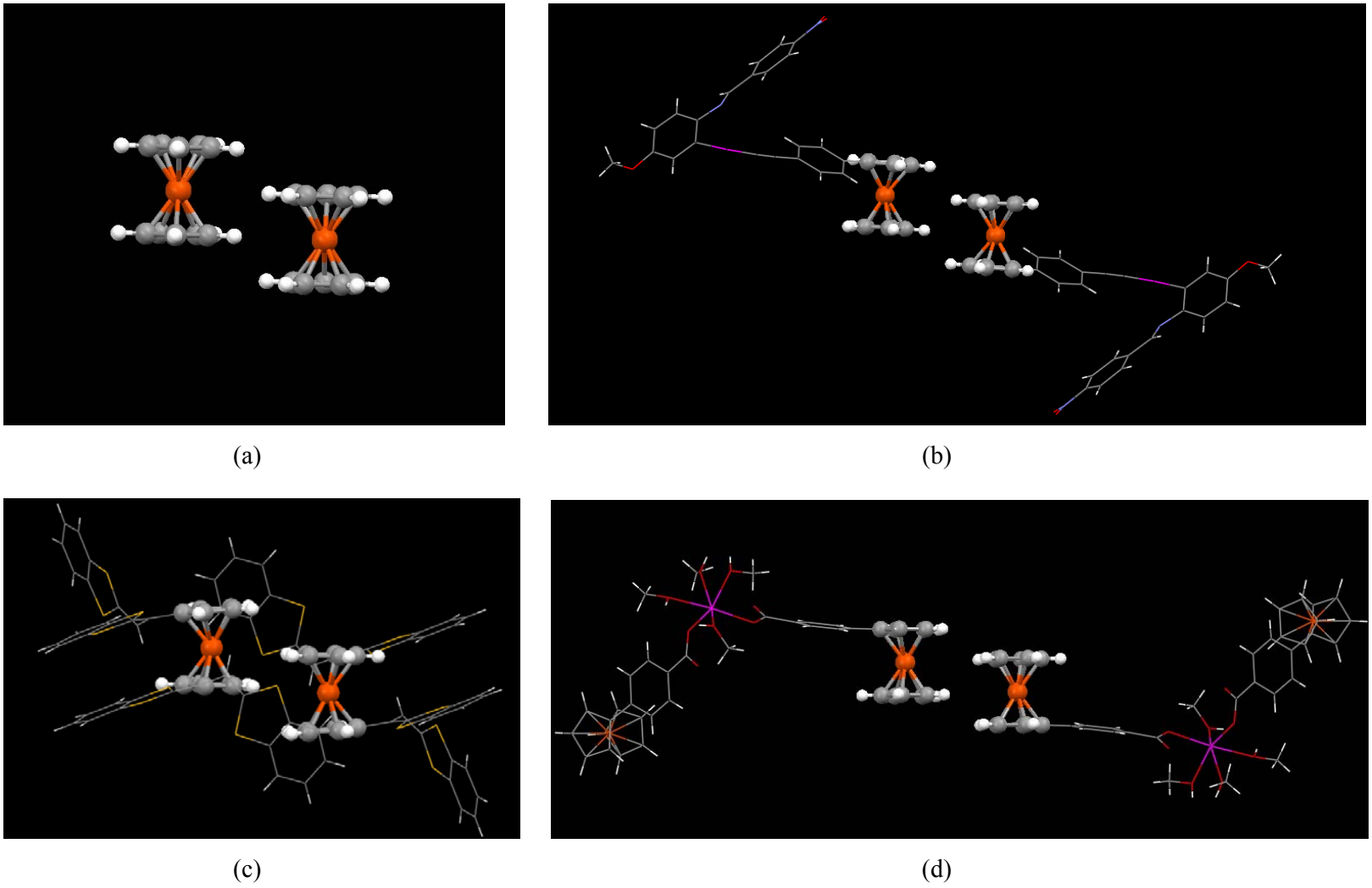


Fig. S2 Distribution of the geometrical parameters describing FcD for all crystal structures containing Fc moieties regardless the manner of their substitution.



(a) (b)

(c) (d)

Fig. S3 Some examples of Fc dimer arrangement within the crystal structures of: (a) unsubstituted Fc, CSD[1] refcode: FEROCE24[2] and Fc derivatives with complex substituents, CSD[1] refcodes: (b) AXODOG[3]; (c) COMCIR[4] and (d) BOFQIW.[5]

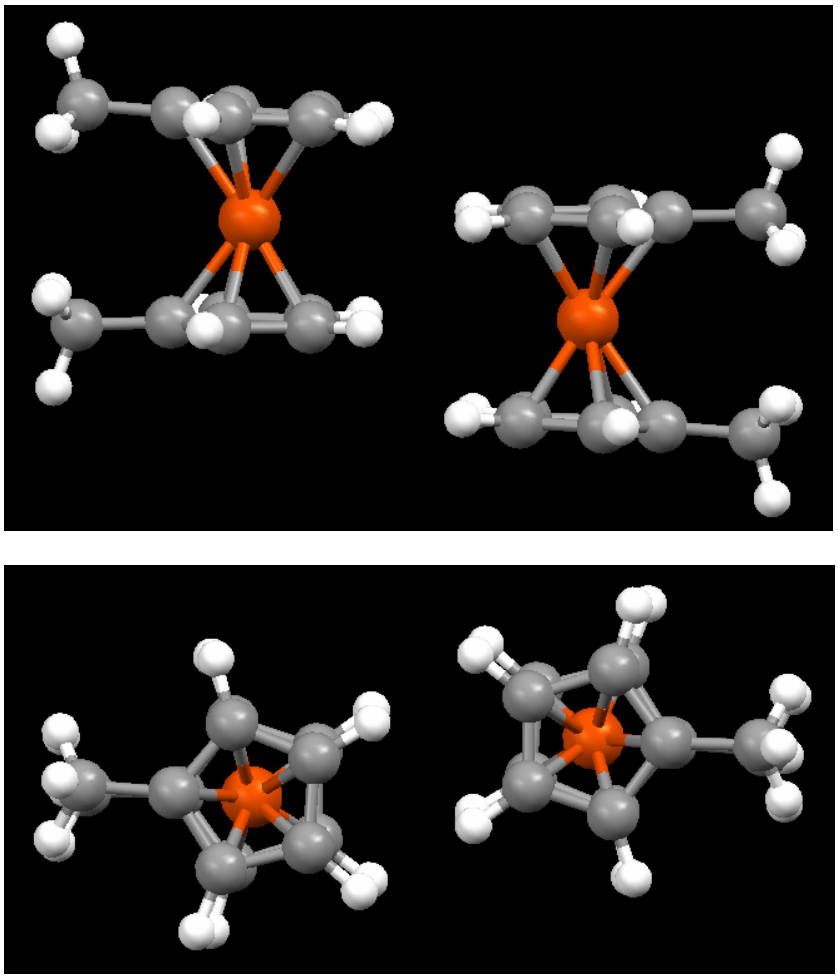


Fig. S4 Crystal structure of 1,1'-dimethyl ferrocene[6] dimer, two orthogonal projections.

Tabele S1 Geometrical parameters of 1,1'-dimethyl ferrocene dimer

Fe1…Cg2 (Å)	5.49
Fe2…Cg1 (Å)	5.49
Fe1−Cg1…Fe2 (°)	89.1
Fe2−Cg2…Fe1 (°)	89.1
Cg1−Fe1…Cg2 (°)	90.9
Cg2−Fe2…Cg1 (°)	90.9
Fe1−Cg1−Fe2−Cg2 (°)	0.0
Fe…H (Å)	3.58

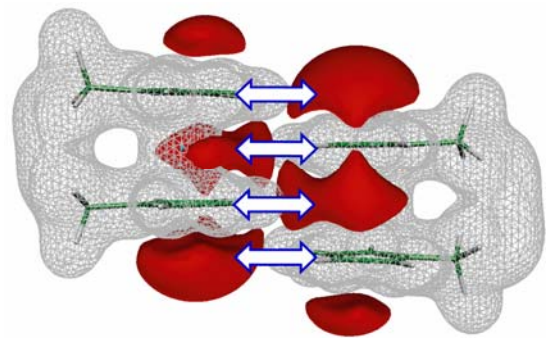
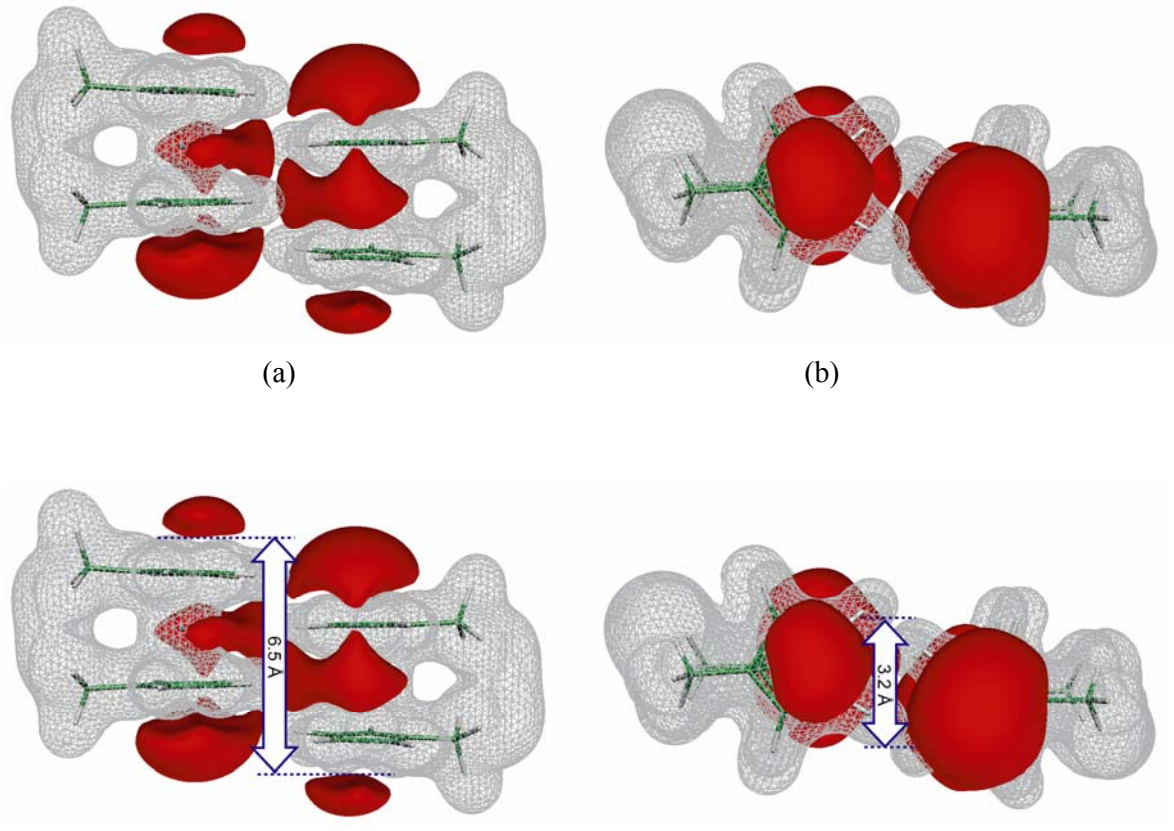


Fig. S5 EP of the dimer derived from experimental charge density data for 1,1'-dimethyl ferrocene[6] (isosurfaces at: −0.055 and +0.055 au, red and grey, respectively). Arrows indicate the regions of the electrostatic complementarily within the dimer in the crystal structure.



(a) (b)

(c) (d)

Fig. S6 (a) and (b) two orthogonal projections of the EP for 1,1'-dimethyl ferrocene dimer derived from the experimental charge density data[1] (isosurfaces as above); (c) and (d) display the (approximate) dimension of the interacting surface.

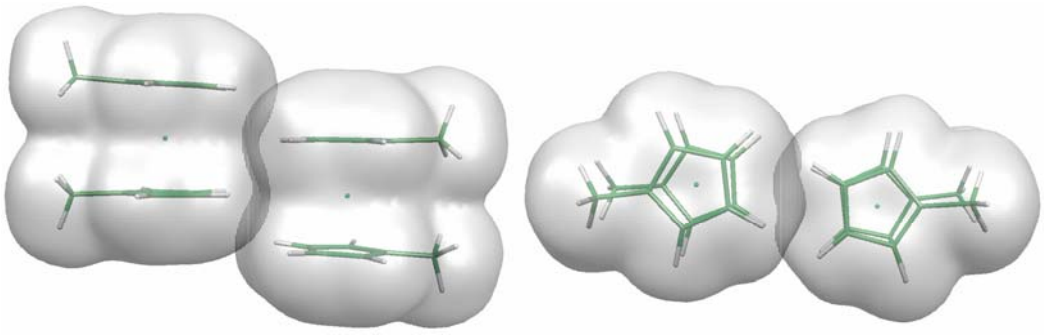


Fig. S7 Two orthogonal projections of the total electron density for 1,1'-dimethyl ferrocene[6] dimer derived from the experimental charge density data. Isosurface at 0.001 au.[7]

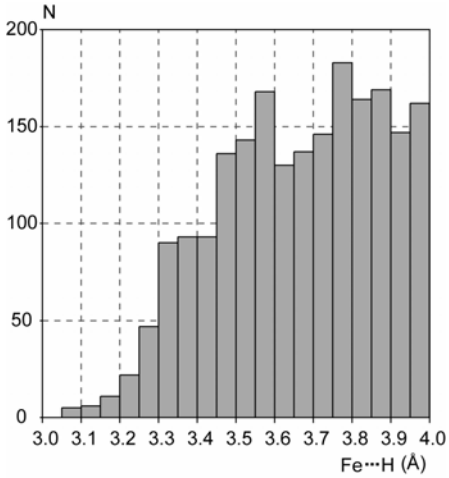


Fig. S8 Distribution of Fe…H distances within FcD in crystal structures containing monosubstituted Fc moieties.

Theoretical calculations. Single-point *ab initio* calculations for 1,1'-dimethyl ferrocene[1] was performed using the Gaussian 03 program.[8] The calculations were carried out for molecule in the gas-phase at the B3LYP/6-31G* level of theory, which according to Zhang *et al.*[9] shows the best agreement with the experimental values for ferrocene. The coordinates used in calculation of the electrostatic properties of 1,1'-dimethyl ferrocene are those obtained from multipole refinement by Makal *et al.*[6], as extracted from CSD.[1]

References:

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