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SUPPORTING INFORMATION

Charge transfer modulation in Charge Transfer co-crystal driven by crystal structure morphology

Federica Solano[1], Paolo Inaudi[1]*, Ornella Abollino[1], Agnese Giacomino[1], Mario Chiesa[2], Enrico Salvadori[2], Gabriele Kociok-Kohn[3], Enrico da Como[4]*, Tommaso Salzillo[5], Claudio Fontanesi[6,7]*

[1] *Department of Drug Science and Technology, University of Torino, Via Giuria 9, Torino, Italy*

[2] *Department of Chemistry, University of Torino, Via Giuria 5, Torino, Italy*

[3] *Material and Chemical Characterization Facility (MC2), University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*

[4] *Department of Physics, University of Bath, BA2 7AY, United Kingdom*

[5] *Department of Industrial Chemistry, "Toso Montanari", University of Bologna, Viale del Risorgimento 4, Bologna, Italy.*

[6] *University of Modena and Reggio Emilia, DIEF, via Vivarelli 10, 41125 Modena, Italy*

[7] *National Interuniversity Consortium of Materials Science and Technology (INSTM), Via G. Giusti 9, 50121 Firenze (FI), Italy.*

Content

1. Estimation of HOMO and LUMO from E_{ONSET}

Energy of HOMO and LUMO were calculated from E_{ONSET} as[1]

HOMO = $-Eonset,ox$ (4,8 – $Eonset,ox\ fc$) [eV]

LUMO = $-E\ onset,red$ (4,8 – $Eonset,ox\ fc$) [eV]

2. Additional electrochemical results

CVs of PE:F4 co-crystals in the 20 50 100 mV s^{-1} scan rate.

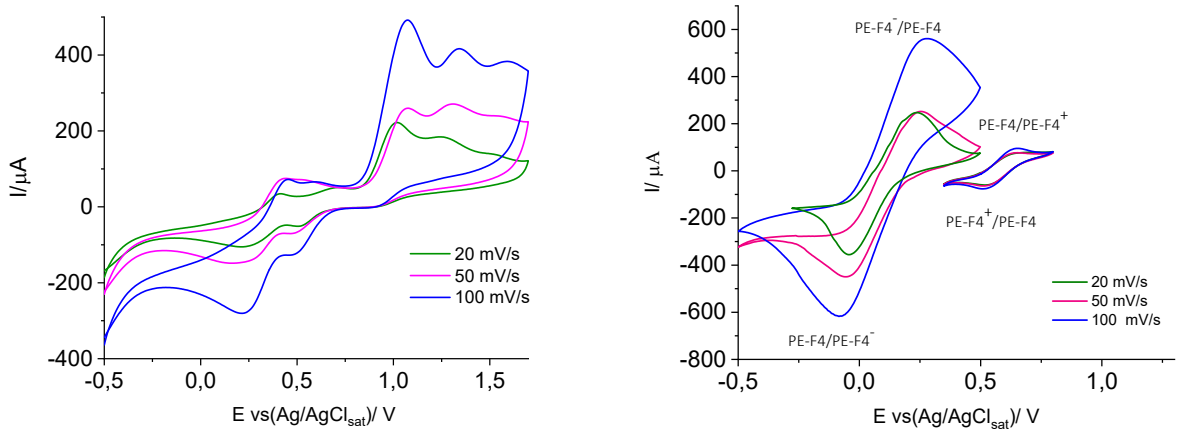

Figure 1S. *CVs of DB:F4 co-crystal in the 0.0 to 1.6 V potential range b)CVs of PE:F4 co-crystal recorded starting from the OCP to anodic and cathodic scans. 20 50 100 mV s^{-1} scan rate.*

Table 1S. *Oxidation-reductive processes of PE:F4 co-crystal*

$PE{:}F4_{(solid)} + e^-$	⇄	$PE{:}F4^-_{(solid)}$	E_p^1
$PE{:}F4_{(solid)}$	⇄	$PE{:}DB^+_{(solid)} + e^-$	E_p^2

Table 2S. *E, ΔE, $E_{1/2}$ to 20, 50, 100 mV s^{-1} of PE:F4 co-crystal*

Scan rate	*E (V)*	*ΔE (V)*	*$E_{1/2}$ (V)*
20 mV s^{-1}			
E_{pa}^1 E_{pc}^1	0.238 -0.046	0.284	0.096
E_{pa}^2 E_{pc}^2	0.640 0.533	0.107	0.587

50 mV s^{-1}			
E_{pa}^{1} E_{pc}^{1}	0.252 -0.046	0.298	0.103
E_{pa}^{2} E_{pc}^{2}	0.640 0.524	0.116	0.582
100 mV s^{-1}			
E_{pa}^{1} E_{pc}^{1}	0.278 -0.077	0.355	0.101
E_{pa}^{2} E_{pc}^{2}	0.645 0.520	0.125	0.583

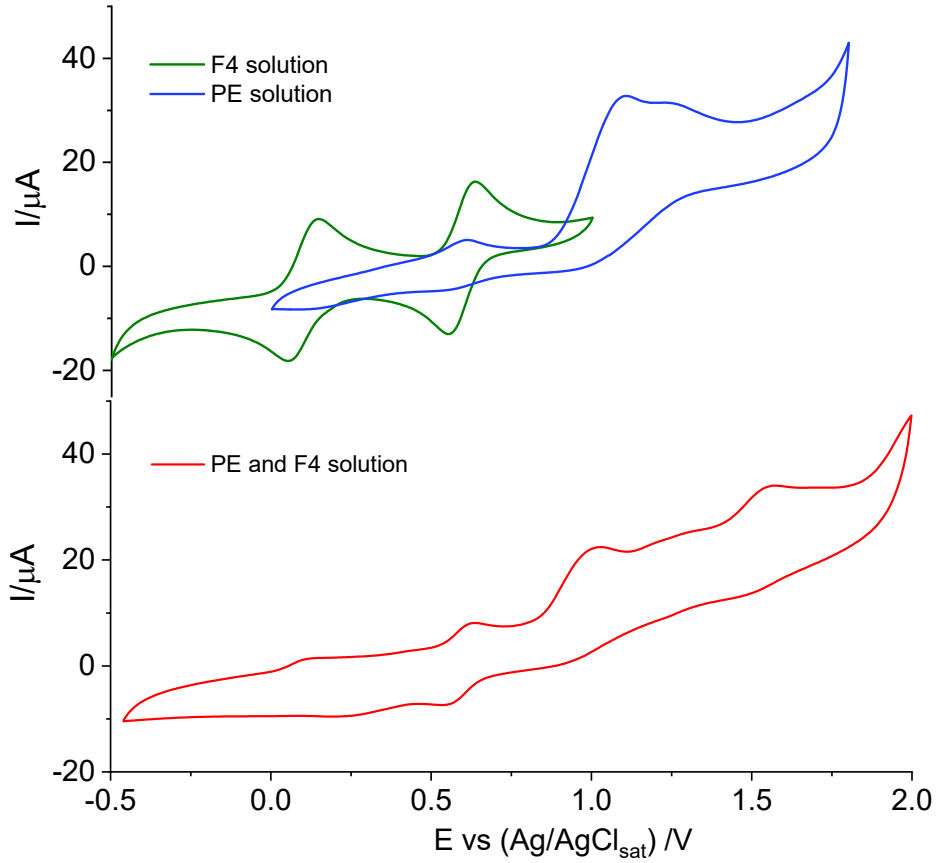

Figure 2S. *CVs of the 1mM F4 and 1mM PE compounds in 0.1 M $TBAPF_6$ ACN solution. Figure 9b) CV of the 0.1 mM PE and 0.1mM F4 simultaneously in solution. WE: GCE, RE: Ag/AgCl/KCl_{sat} , CE: Pt wire. 50 mV s^{-1} is the potential scan rate.*

3. Theoretical results

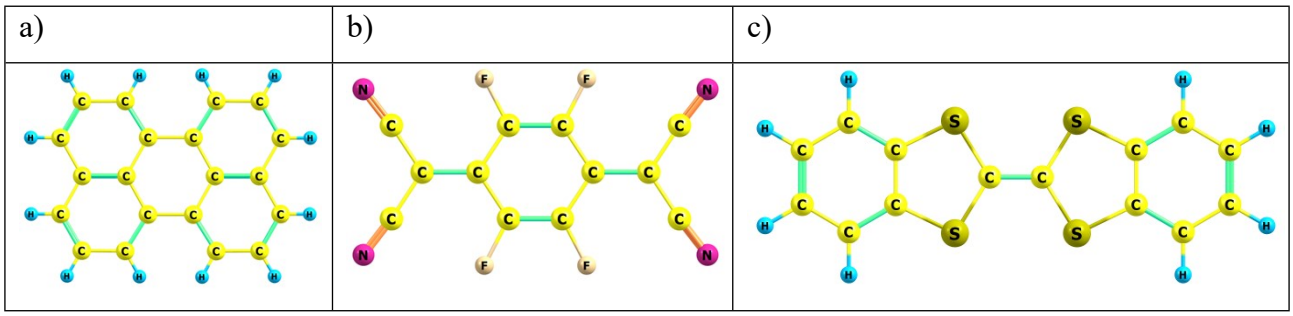

Figure 3S. *Chemical structures. a) perylene b) 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane 98% purity (F4) c) Dibenzotetrathiafulvalene (DBTTF).*

3.1 Plane wave ELF 2D sections

PE:F4 triclinic k-point sampling path selection

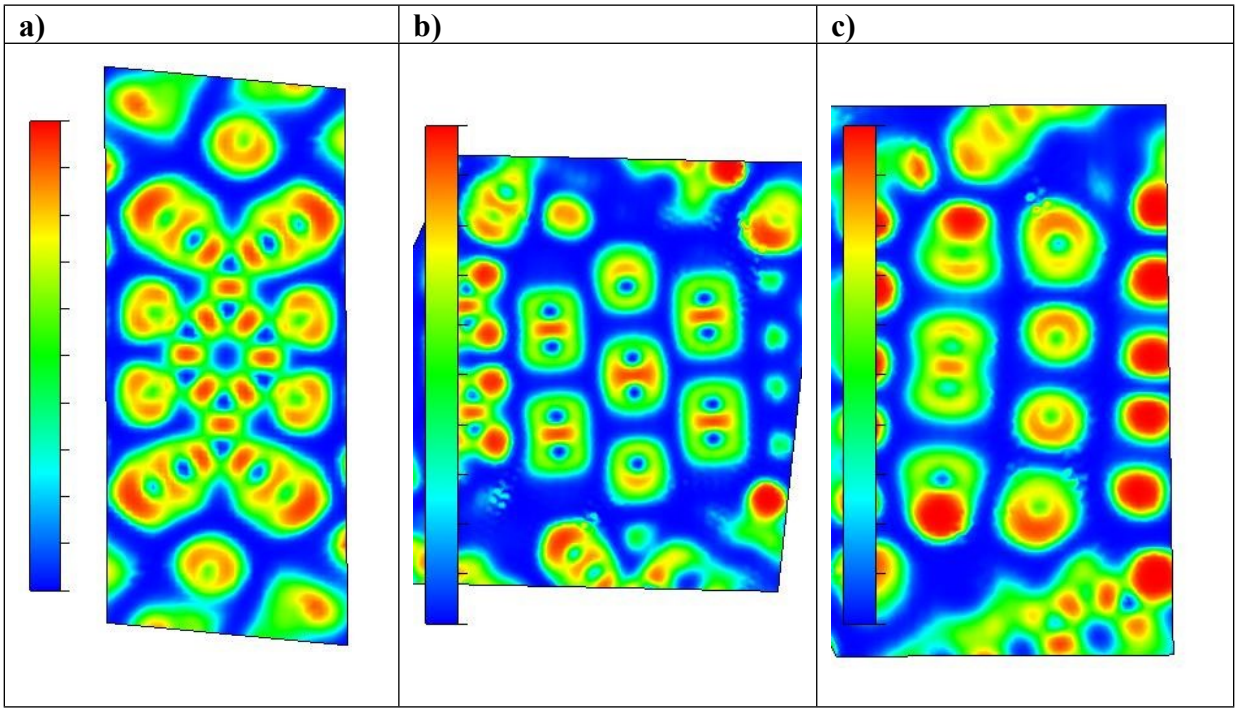

Figure 4S. *2D projections of ELF, relevant to the 3D plot Figure 4 main manuscript. Colour scale: blue low electron density, red high electron density. a) projection coplanar with the F4 molecule b) projection orthogonal to the F4 aromatic plane, carbon atoms only c) projection orthogonal to the F4 aromatic plane, passing through fluorine and carbon atoms.*[3]

3.2 Localized Orbitals

For the sake of comparison, theoretical results obtained by using localized orbitals are here reported too. Theoretical calculations were carried out using a cluster strategy. In particular, we selected a cluster constituted by a total of three molecules: two PE and one F4, Figure 5Sa. The geometry of the cluster was maintained fixed and corresponds exactly to the one obtained by the analysis of the experimental X-ray data [4], Figure 4b shows the molecular graphical representation of the PE:F4 superstructure, van der Waals radii, within the co-crystal.

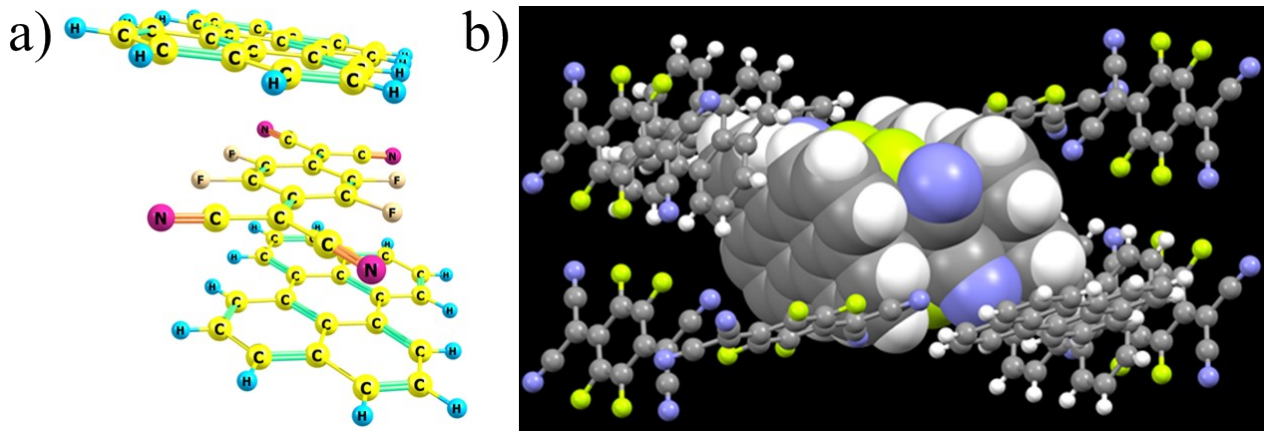

Figure 5S. a) Graphical representation of the PE:F4 superstructure used in the theoretical calculations, atomic coordinates were obtained from the relevant experimental, X-ray, co-crystal geometries. b) X-ray, co-crystal geometry, van der Waals radii, highlights the PE:F4 superstructure used in the calculations with the crystal geometry (reproduced with permission from [4])

Table III summarizes the theoretical values of HOMO, LUMO and band gap energies, as well as total molecular electronic energy and atomic Mulliken net charge. The latter is factorized in terms of net charge found on each molecule forming the cluster, the latter is neutral as a whole. Indeed, in CT co-crystal the donor-acceptor net charge values are of great interest. The "degree" of intermolecular charge transfer can be made quantitative exploiting the Mulliken electron density decomposition scheme. In the PE:F4 co-crystal cluster the singlet is definitively the most stable electronic state, the triplet and quintet are found 26 and 73 kcal mol-1 higher in energy, respectively. Thus, the PE:F4 electronic ground state has essentially singlet character, the relevant net charge on the donor and acceptor molecules is about -0.3 on the F4 and +0.15 on each PE molecule. The latter result is consistent with previously published results concerning PE:F4 co-crystals family.[4] The variation in the frontier orbital energies parallels the outcome obtained in terms of intermolecular charge transfer. A much more prominent charge transfer was found in the DB:F4 co-crystal, as recently reported in the literature.[5] Indeed, the variation of the electronic MO energies in the PE:F4 co-crystal is found smaller if compared to the results obtained in the case of DB:F4.[5] The trend in molecular orbital energies obtained by theoretical calculations match in a semi-quantitative way the experimental

values yielded by the analysis of the pristine and solid-state co-crystal CVs. Please compare the experimental values shown in Table I with the theoretical Table III and Table IV values.

Table IIIS. PE:F4 cluster. LUMO, HOMO, Mulliken net charge, energy stability values for the singlet, triplet and quintet electronic state multiplicity, UCAM-B3LYP/6-31G* level of the theory. Compare Figure 4B for the relevant geometry.			
	Singlet	Triplet	quintet
	Vacuum	Vacuum	Vacuum
$LUMO\ /\ eV$	–3.1470	–4.4270	–3.5502
$HOMO\ /\ eV$	–6.3275	–5.3405	–3.7470
$LUMO - HOMO\ /\ eV$	+3.1804	+0.9134	+0.1967
$Charge\ F4\ /\ electrons$	–0.28846	–0.9884	–0.9755
$Energy\ /\ kcal\ mol^{-1}$	0	+26.5	+72.9

A peculiar picture emerges in the case of the PE:F4. Due to an initial less pronounced charge transfer, the electron transfer process leads to the formation of a F4 anion, with each single PE unit much less (50%) positively charged. PE molecules of neighbour unit cell form a kind of herringbone continuous sub-structure which is able to conduct the current with great efficiency. The opposite holds for the oxidation process, here the major net charge variation is due to the PE, in the neutral co-crystal the F4 is weakly negative, now the charge is largely localized on the PE leading to a less efficient electrical conductor. In fact, in the PE:F4 the HOMO is localized on the PE and the LUMO on the F4, this at variance of the DB:F4. All in all, the theoretical results give due reason to the simply reasonable conclusions inferred by the analysis of the experimental CVs, vide-supra.

Table IVS. Mulliken net charges UCAM-B3LYP/6-31G* level of the theory.					
			variation		variation
	neutral	anion	$0 \rightarrow anion$	cation	$0 \rightarrow cation$
Charge PE 1	0.144219	0.009917	-0.1343	0.708971	0.564752
Charge PE 2	0.144243	0.009882	-0.1344	0.708971	0.564728
Charge PE both	0.28846	0.019799	-0.2687	1.418513	1.130053
Charge F4	-0.28846	-1.0198	-0.7313	-0.41851	-0.13005

Table VS. Total electronic energies for three state multiplicity values: B3LYP, MP2(FC) and pure HF level of theory.

	Relative energy / kcal mol^{-1} State multiplicity			a.u	a.u	a.u
	1	3	5			
B3LYP no_slv	0	0.05046463	0.15219112	-2613.90311	-2613.85265	-2613.75092
B3LYP slv	0	0.05286564	0.09639076	-2613.92501	-2613.87214	-2613.82862
MP2	0	0.41452951	0.45304633	-2606.18507	-2605.77054	-2605.73202
HF	0	-0.08603449	-0.00247924	-2598.26467	-2598.35070	-2598.26715

Table VIS. HOMO, LUMO and HOMO-LUMO gap energies, singlet and triplet states: B3LYP, MP2(FC) and pure HF level of theory.

	Multiplicity = 1			Multiplicity = 3		
	HOMO	LUMO	$\Delta_{(HOMO,LUMO)}$	HOMO	LUMO	$\Delta_{(HOMO,LUMO)}$
	eV					
B3LYP no_slv	-5.25211092	-3.814794204	1.437316712	-4.96557277	-5.30843893	-0.34286616
B3LYP slv	-5.25809747	-3.957382988	1.30071448	-5.01237672	-5.48449798	-0.47212126
MP2	-6.58847259	-1.41092146	5.177551132	-7.81762056	-1.93637746	5.881243108
HF	-6.58847259	-1.41092146	5.177551132	-7.81762056	-1.93637746	5.881243108

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In the following the cif file corresponding to the full relaxation (molecular coordinates and lattice vectors), plane waves pbc (2731.97 Å^3 the cell volume):

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

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F2	1.0	0.305508	0.424036	0.008316	Biso	1.000000	F
F3	1.0	0.323857	0.572811	0.066712	Biso	1.000000	F
F4	1.0	0.676143	0.427189	0.933288	Biso	1.000000	F
F5	1.0	0.173376	0.419112	0.506406	Biso	1.000000	F
F6	1.0	0.826624	0.580888	0.493594	Biso	1.000000	F
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C81	1.0	0.007641	0.559596	0.181373	Biso	1.000000	C
C82	1.0	0.992359	0.440404	0.818627	Biso	1.000000	C
C83	1.0	0.317993	0.558302	0.226950	Biso	1.000000	C
C84	1.0	0.682007	0.441698	0.773051	Biso	1.000000	C
C85	1.0	0.328944	0.638048	0.257559	Biso	1.000000	C
C86	1.0	0.671056	0.361952	0.742441	Biso	1.000000	C
C87	1.0	0.183328	0.679444	0.250326	Biso	1.000000	C
C88	1.0	0.816672	0.320556	0.749674	Biso	1.000000	C
C89	1.0	0.526508	0.685447	0.415748	Biso	1.000000	C
C90	1.0	0.473492	0.314553	0.584252	Biso	1.000000	C
C91	1.0	0.691408	0.728960	0.410331	Biso	1.000000	C
C92	1.0	0.308592	0.271040	0.589669	Biso	1.000000	C
C93	1.0	0.838519	0.693530	0.372644	Biso	1.000000	C
C94	1.0	0.161481	0.306470	0.627356	Biso	1.000000	C
C95	1.0	0.827228	0.613921	0.340691	Biso	1.000000	C
C96	1.0	0.172772	0.386079	0.659308	Biso	1.000000	C
C97	1.0	0.668847	0.568014	0.344964	Biso	1.000000	C
C98	1.0	0.331153	0.431986	0.655036	Biso	1.000000	C
C99	1.0	0.656416	0.484784	0.312132	Biso	1.000000	C
C100	1.0	0.343584	0.515216	0.687868	Biso	1.000000	C
C101	1.0	0.802159	0.445683	0.274479	Biso	1.000000	C
C102	1.0	0.197841	0.554317	0.725522	Biso	1.000000	C

C103	1.0	0.789366	0.365908	0.243788	Biso	1.000000	C
C104	1.0	0.210634	0.634092	0.756212	Biso	1.000000	C
C105	1.0	0.630560	0.323029	0.250088	Biso	1.000000	C
C106	1.0	0.369440	0.676970	0.749912	Biso	1.000000	C
C107	1.0	0.478044	0.359691	0.287237	Biso	1.000000	C
C108	1.0	0.521955	0.640309	0.712763	Biso	1.000000	C
C109	1.0	0.313466	0.316734	0.293967	Biso	1.000000	C
C110	1.0	0.686534	0.683266	0.706033	Biso	1.000000	C
C111	1.0	0.163318	0.352804	0.329433	Biso	1.000000	C
C112	1.0	0.836682	0.647196	0.670567	Biso	1.000000	C
C113	1.0	0.174311	0.432466	0.359529	Biso	1.000000	C
C114	1.0	0.825689	0.567534	0.640471	Biso	1.000000	C
C115	1.0	0.334091	0.477797	0.355164	Biso	1.000000	C
C116	1.0	0.665909	0.522203	0.644836	Biso	1.000000	C
C117	1.0	0.489916	0.441322	0.318442	Biso	1.000000	C
C118	1.0	0.510084	0.558678	0.681558	Biso	1.000000	C
C119	1.0	0.346562	0.560697	0.387949	Biso	1.000000	C
C120	1.0	0.653438	0.439303	0.612051	Biso	1.000000	C
C121	1.0	0.514223	0.604070	0.382705	Biso	1.000000	C
C122	1.0	0.485777	0.395930	0.617295	Biso	1.000000	C
C123	1.0	0.199142	0.599278	0.425305	Biso	1.000000	C
C124	1.0	0.800858	0.400722	0.574695	Biso	1.000000	C
C125	1.0	0.212111	0.678606	0.458073	Biso	1.000000	C
C126	1.0	0.787889	0.321394	0.541927	Biso	1.000000	C
C127	1.0	0.374214	0.721417	0.453761	Biso	1.000000	C
C128	1.0	0.625786	0.278583	0.546239	Biso	1.000000	C
C129	1.0	0.762544	0.033238	0.132762	Biso	1.000000	C
C130	1.0	0.237456	0.966762	0.867238	Biso	1.000000	C
C131	1.0	0.680611	0.977972	0.074421	Biso	1.000000	C
C132	1.0	0.319389	0.022028	0.925579	Biso	1.000000	C
C133	1.0	0.599366	0.909035	0.073847	Biso	1.000000	C
C134	1.0	0.400634	0.090965	0.926153	Biso	1.000000	C
C135	1.0	0.595410	0.893498	0.131124	Biso	1.000000	C
C136	1.0	0.404590	0.106502	0.868876	Biso	1.000000	C
C137	1.0	0.675634	0.946066	0.190152	Biso	1.000000	C
C138	1.0	0.324366	0.053934	0.809848	Biso	1.000000	C
C139	1.0	0.676331	0.929707	0.249672	Biso	1.000000	C
C140	1.0	0.323669	0.070293	0.750328	Biso	1.000000	C
C141	1.0	0.598001	0.859989	0.251122	Biso	1.000000	C
C142	1.0	0.401999	0.140011	0.748878	Biso	1.000000	C
C143	1.0	0.596273	0.845544	0.308835	Biso	1.000000	C
C144	1.0	0.403727	0.154456	0.691165	Biso	1.000000	C

C145	1.0	0.671761	0.899995	0.366575	Biso	1.000000	C
C146	1.0	0.328239	0.100005	0.633425	Biso	1.000000	C
C147	1.0	0.754139	0.970609	0.367528	Biso	1.000000	C
C148	1.0	0.245861	0.029391	0.632472	Biso	1.000000	C
C149	1.0	0.756918	0.985973	0.308571	Biso	1.000000	C
C150	1.0	0.243082	0.014027	0.691429	Biso	1.000000	C
C151	1.0	0.832093	0.026543	0.426240	Biso	1.000000	C
C152	1.0	0.167907	0.973457	0.573761	Biso	1.000000	C
C153	1.0	0.909659	0.096118	0.427015	Biso	1.000000	C
C154	1.0	0.090341	0.903882	0.572985	Biso	1.000000	C
C155	1.0	0.912731	0.111343	0.369623	Biso	1.000000	C
C156	1.0	0.087269	0.888657	0.630377	Biso	1.000000	C
C157	1.0	0.838998	0.057718	0.310068	Biso	1.000000	C
C158	1.0	0.161002	0.942282	0.689932	Biso	1.000000	C
C159	1.0	0.843686	0.073167	0.250176	Biso	1.000000	C
C160	1.0	0.156314	0.926833	0.749824	Biso	1.000000	C
C161	1.0	0.760475	0.017464	0.191493	Biso	1.000000	C
C162	1.0	0.239525	0.982536	0.808507	Biso	1.000000	C
C163	1.0	0.928835	0.141629	0.248182	Biso	1.000000	C
C164	1.0	0.071165	0.858371	0.751818	Biso	1.000000	C
C165	1.0	0.931240	0.156422	0.190682	Biso	1.000000	C
C166	1.0	0.068760	0.843578	0.809318	Biso	1.000000	C
C167	1.0	0.848908	0.103229	0.133450	Biso	1.000000	C
C168	1.0	0.151092	0.896771	0.866550	Biso	1.000000	C
H1	1.0	0.880771	0.744778	0.228253	Biso	1.000000	H
H2	1.0	0.119229	0.255222	0.771747	Biso	1.000000	H
H3	1.0	0.590498	0.676588	0.163045	Biso	1.000000	H
H4	1.0	0.409502	0.323412	0.836955	Biso	1.000000	H
H5	1.0	0.565679	0.537240	0.111554	Biso	1.000000	H
H6	1.0	0.434321	0.462760	0.888446	Biso	1.000000	H
H7	1.0	0.550833	0.428842	0.068959	Biso	1.000000	H
H8	1.0	0.449167	0.571158	0.931041	Biso	1.000000	H
H9	1.0	0.533362	0.290204	0.011896	Biso	1.000000	H
H10	1.0	0.466638	0.709796	0.988104	Biso	1.000000	H
H11	1.0	0.803474	0.215643	0.021810	Biso	1.000000	H
H12	1.0	0.196526	0.784357	0.978190	Biso	1.000000	H
H13	1.0	0.114046	0.211371	0.066098	Biso	1.000000	H
H14	1.0	0.885954	0.788629	0.933902	Biso	1.000000	H
H15	1.0	0.397008	0.277882	0.134173	Biso	1.000000	H
H16	1.0	0.602992	0.722118	0.865827	Biso	1.000000	H
H17	1.0	0.422595	0.417618	0.189212	Biso	1.000000	H
H18	1.0	0.577405	0.582382	0.810788	Biso	1.000000	H

H19	1.0	0.436368	0.527918	0.233613	Biso	1.000000	H
H20	1.0	0.563632	0.472082	0.766387	Biso	1.000000	H
H21	1.0	0.454626	0.666777	0.287097	Biso	1.000000	H
H22	1.0	0.545374	0.333223	0.712903	Biso	1.000000	H
H23	1.0	0.190313	0.741486	0.274241	Biso	1.000000	H
H24	1.0	0.809687	0.258514	0.725759	Biso	1.000000	H
H25	1.0	0.700083	0.790599	0.436899	Biso	1.000000	H
H26	1.0	0.299917	0.209401	0.563101	Biso	1.000000	H
H27	1.0	0.964588	0.727592	0.368505	Biso	1.000000	H
H28	1.0	0.035412	0.272408	0.631495	Biso	1.000000	H
H29	1.0	0.947115	0.587970	0.312261	Biso	1.000000	H
H30	1.0	0.052885	0.412030	0.687739	Biso	1.000000	H
H31	1.0	0.930567	0.477190	0.268616	Biso	1.000000	H
H32	1.0	0.069433	0.522810	0.731384	Biso	1.000000	H
H33	1.0	0.907112	0.338147	0.215071	Biso	1.000000	H
H34	1.0	0.092888	0.661853	0.784929	Biso	1.000000	H
H35	1.0	0.620193	0.260894	0.226492	Biso	1.000000	H
H36	1.0	0.379807	0.739106	0.773508	Biso	1.000000	H
H37	1.0	0.307886	0.254700	0.270226	Biso	1.000000	H
H38	1.0	0.692114	0.745300	0.729774	Biso	1.000000	H
H39	1.0	0.036248	0.320046	0.334991	Biso	1.000000	H
H40	1.0	0.963752	0.679954	0.665009	Biso	1.000000	H
H41	1.0	0.054275	0.459083	0.387089	Biso	1.000000	H
H42	1.0	0.945725	0.540917	0.612911	Biso	1.000000	H
H43	1.0	0.070126	0.567352	0.429656	Biso	1.000000	H
H44	1.0	0.929874	0.432648	0.570344	Biso	1.000000	H
H45	1.0	0.094574	0.706060	0.487357	Biso	1.000000	H
H46	1.0	0.905426	0.293940	0.512643	Biso	1.000000	H
H47	1.0	0.387152	0.783417	0.478971	Biso	1.000000	H
H48	1.0	0.612848	0.216583	0.521029	Biso	1.000000	H
H49	1.0	0.684634	0.990562	0.029974	Biso	1.000000	H
H50	1.0	0.315366	0.009438	0.970026	Biso	1.000000	H
H51	1.0	0.539647	0.866368	0.028417	Biso	1.000000	H
H52	1.0	0.460353	0.133632	0.971583	Biso	1.000000	H
H53	1.0	0.530026	0.838753	0.128767	Biso	1.000000	H
H54	1.0	0.469974	0.161247	0.871233	Biso	1.000000	H
H55	1.0	0.533469	0.816571	0.207043	Biso	1.000000	H
H56	1.0	0.466531	0.183429	0.792957	Biso	1.000000	H
H57	1.0	0.532959	0.791261	0.308614	Biso	1.000000	H
H58	1.0	0.467041	0.208739	0.691386	Biso	1.000000	H
H59	1.0	0.666214	0.889976	0.412198	Biso	1.000000	H
H60	1.0	0.333786	0.110024	0.587802	Biso	1.000000	H

H61	1.0	0.827945	0.013996	0.470725	Biso	1.000000 H
H62	1.0	0.172055	0.986004	0.529275	Biso	1.000000 H
H63	1.0	0.970283	0.139281	0.472053	Biso	1.000000 H
H64	1.0	0.029717	0.860719	0.527947	Biso	1.000000 H
H65	1.0	0.973716	0.166935	0.372833	Biso	1.000000 H
H66	1.0	0.026284	0.833065	0.627167	Biso	1.000000 H
H67	1.0	0.991973	0.184594	0.292613	Biso	1.000000 H
H68	1.0	0.008027	0.815406	0.707387	Biso	1.000000 H
H69	1.0	0.000423	0.209713	0.190541	Biso	1.000000 H
H70	1.0	-0.000423	0.790287	0.809459	Biso	1.000000 H
H71	1.0	0.851931	0.113864	0.088052	Biso	1.000000 H
H72	1.0	0.148069	0.886136	0.911948	Biso	1.000000 H