FOUNDATIONS
ADVANCES

Volume 77 (2021)

Supporting information for article:

On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model. II. Evaluation of the properties in an infinite crystal

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Supporting information

Table S1 Crystallographic data for the benchmark systems.

	ACG[1]	**BENZ**[2]	**LAC**[3]	**LDOPA**[4]	**PARA**[5]
CSD code	ACYGLY11	BENZEN	YILLAG	LDOPAS03	HXACAN13
Formula	$C_4H_7NO_3$	C_6H_6	$C_3H_6O_3$	$C_9H_{11}NO_4$	$C_8H_9NO_2$
Space group	$P2_1/c$	$Pbca$	$P2_12_12_1$	$P2_1$	$P2_1/a$
a	4.859	7.440	5.490	13.619	12.667
b (Å)	11.546	9.550	8.422	5.232	9.166
c	9.811	6.920	9.345	6.062	7.073
α	90	90	90	90	90
β (°)	97.060	90	90	97.56	115.51
γ	90	90	90	90	90
V (Å^3)	546.2	491.7	432.1	428.2	741.2
Z	4	4	4	2	4

	ABA[6]	**ALA**[7]	**GLY**[8]	**SER**[9]	**VAL**[10]
CSD code	GAMBUT02	LALNIN03	GLYCIN85	LSERIN01	VALIDL02
Formula	$C_4H_9NO_2$	$C_3H_7NO_2$	$C_2H_5NO_2$	$C_3H_7NO_3$	$C_2H_{11}NO_2$
Space group	$P2_1/a$	$P2_12_12_1$	$P2_1/n$	$P2_12_12_1$	$P\bar{1}$
a	8.214	5.928	5.087	8.599	5.222
b (Å)	10.000	12.260	11.773	9.348	5.406
c	7.208	5.794	5.460	5.618	10.838
α	90	90	90	90	90.89
β (°)	110.59	90	111.99	90	92.34
γ	90	90	90	90	110.02
V (Å^3)	554.2	421.1	303.2	451.6	287.1
Z	4	4	4	4	2

	FORM[11]
CSD code	FORMAM02
Formula	CH_3NO
Space group	$P2_1/n$
a	3.604
b (Å)	9.041
c	6.994
α	90
β (°)	100.50
γ	90
V (Å^3)	224.1
Z	4

[1] Mackay, 1975; standard crystallographic settings, originally reported unit cell is 4.859 Å, 11.546 Å, 14.633 Å, 90°, 138.29°, 90°.

[2] Bacon, Curry & Wilson, 1964

[3] Schouten, Kanters & Krieken, 1994

[4] Howard *et al.*, 1995

[5] Wilson, 2000

[6] Weber, Craven & McMullan, 1983

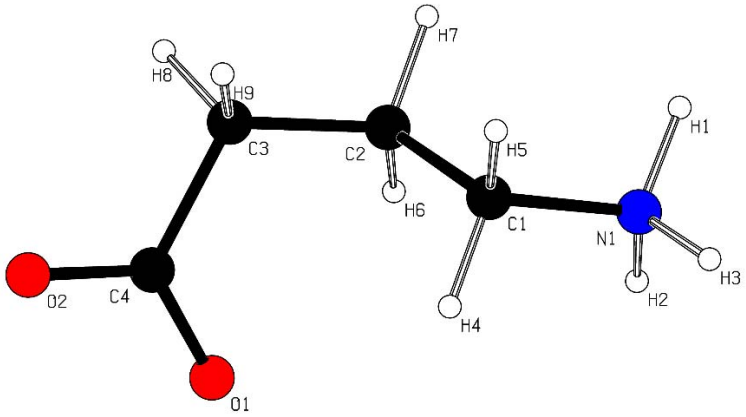
[7] Destro, Marsh & Bianchi, 1988

[8] Destro *et al.*, 2000

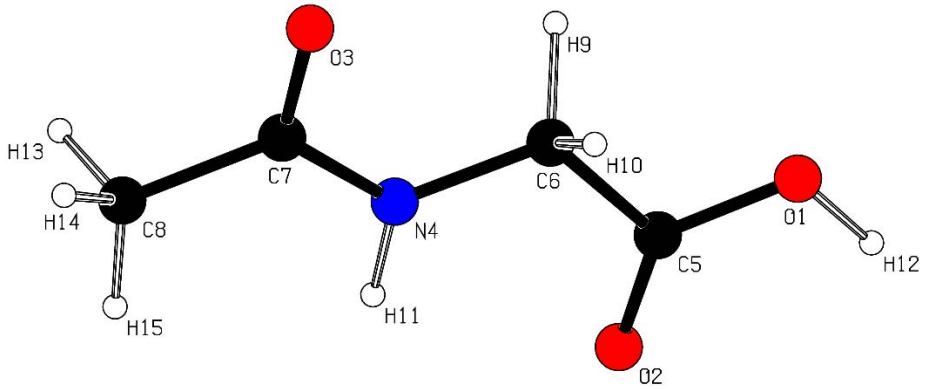
[9] Kistenmacher, Rand & Marsh, 1974

[10] Dalhus & Görbitz, 1996

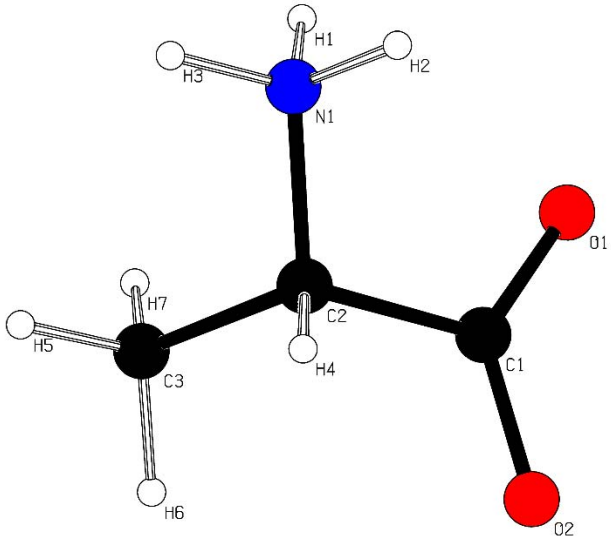
[11] Stevens, 1978



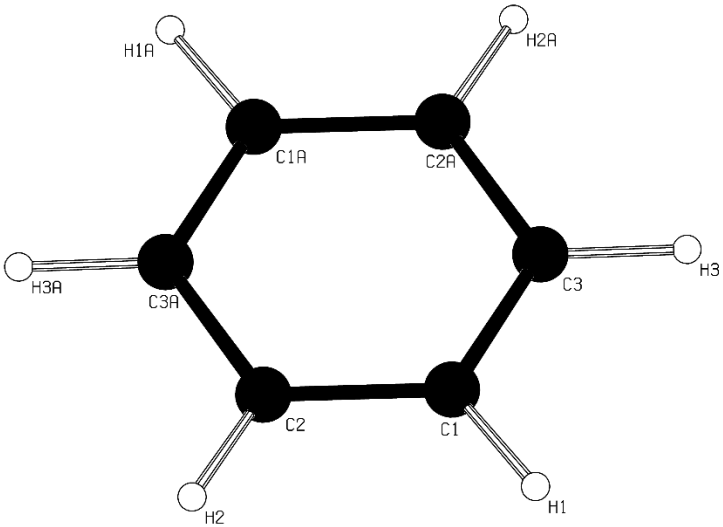
a) ABA



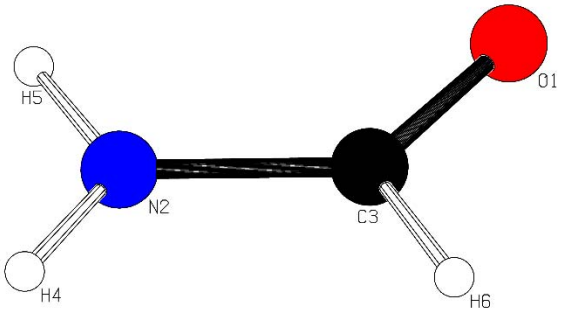
b) ACG



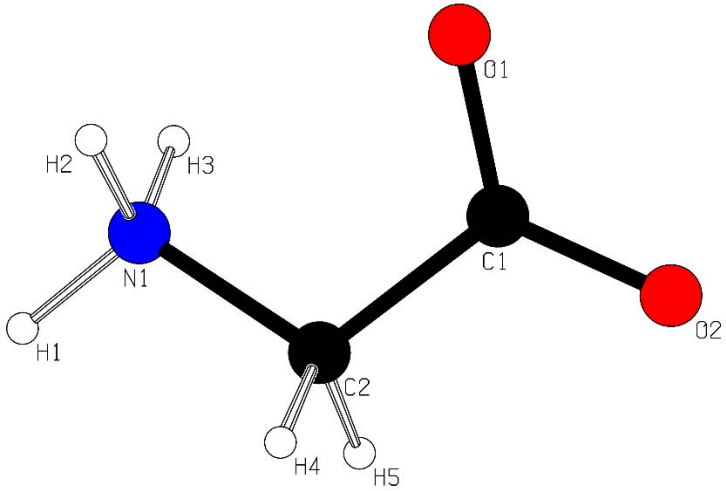
c) ALA



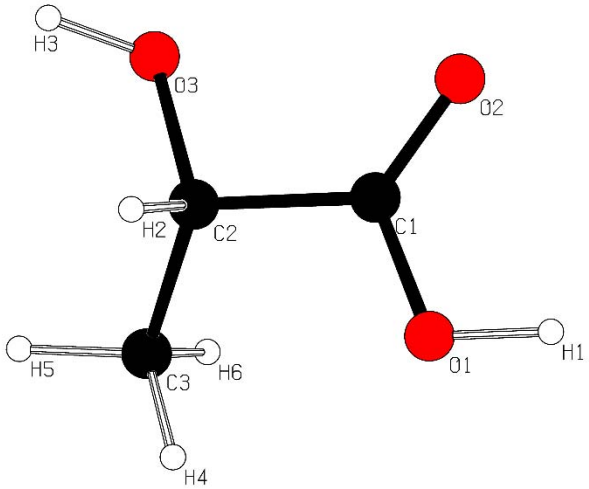
d) BENZ



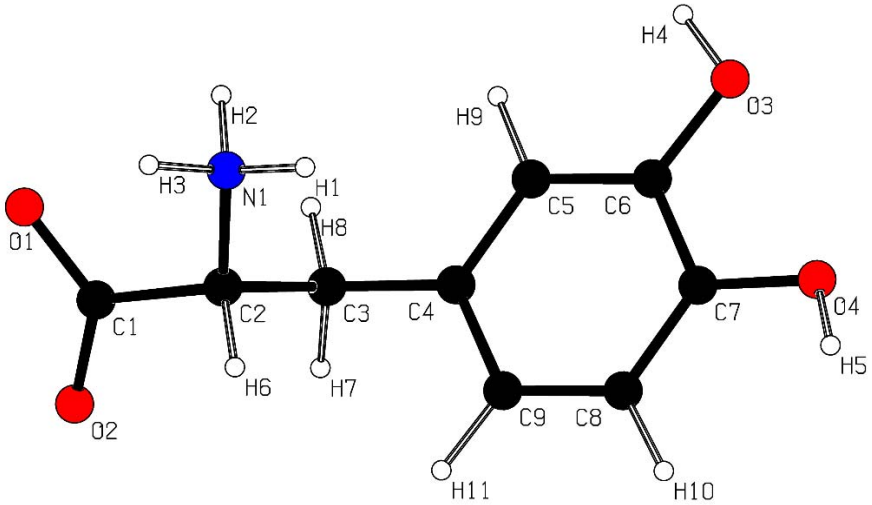
e) FORM



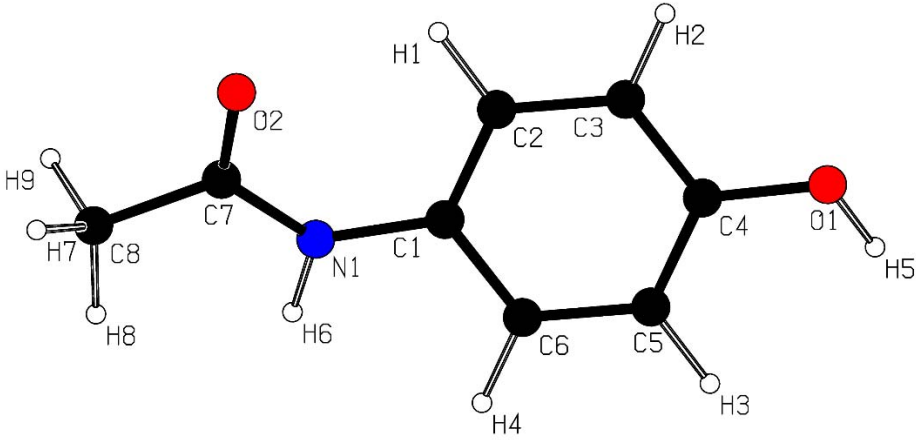
f) GLY



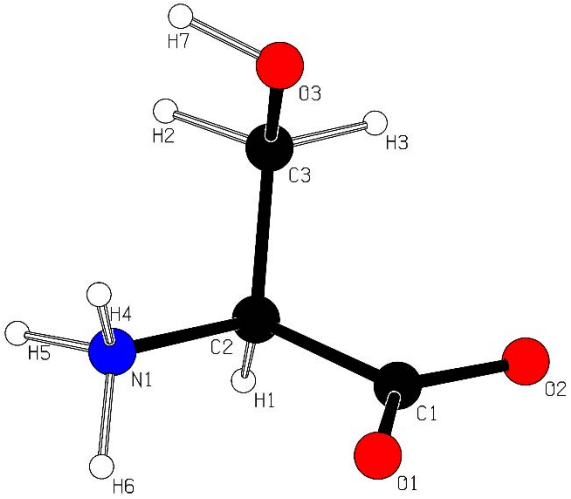
g) LAC



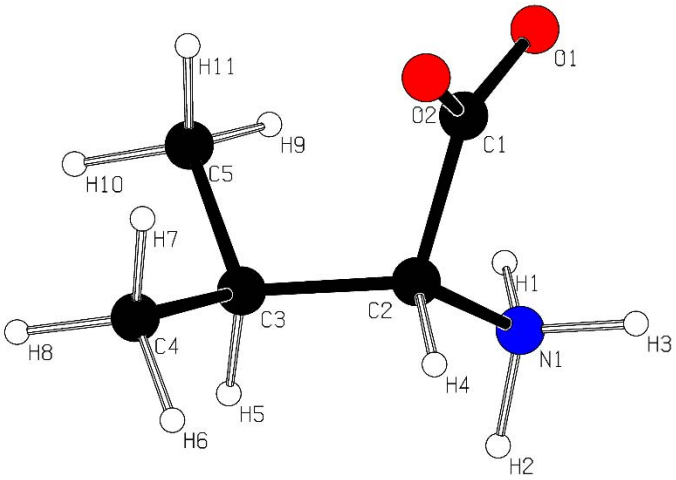
h) LDOPA



i) PARA



j) SER



k) VAL

Figure S1 Molecular structures (Spek, 2003) of the benchmark compounds with atomic labeling.

Table S2 Renormalized Clementi & Roetti (Clementi & Roetti, 1974) atomic wavefunctions for the carbon, nitrogen, oxygen and sulfur atoms.

CARBON 1S(2)2S(2)2P(2), 3P

S-ORBITALS

----- BASIS -----		1S	2S
1S	5.43599	9.326214673861451E-001	-2.081391177861346E-001
1S	9.48256	6.931010905249053E-002	-1.070995460502307E-002
2S	1.05749	8.300013059236350E-004	8.098965671903066E-002
2S	1.52427	-1.760002769187467E-003	7.504468191726948E-001
2S	2.68435	5.590008795317012E-003	3.354885780055265E-001
2S	4.20096	3.820006010395525E-003	-1.476493741766252E-001

P-ORBITALS

----- BASIS ----		2P
2P	0.98073	2.824094774218353E-001
2P	1.44361	5.469689878737340E-001
2P	2.60051	2.319495707942165E-001
2P	6.51003	1.024998103315680E-002

NITROGEN 1S(2)2S(2)2P(3), 4S

S-ORBITALS

----- BASIS ----		1S	2S
1S	6.45739	9.377943527128418E-001	-2.167688043017469E-001
1S	11.17200	5.848964778222875E-002	-8.459953334837750E-003
2S	1.36405	9.299943996832406E-004	1.799090076206453E-001
2S	1.89734	-1.699989762861837E-003	6.741562813491982E-001
2S	3.25291	5.739965434604087E-003	3.129682736647956E-001
2S	5.08238	9.569942370933992E-003	-1.449692003488686E-001

P-ORBITALS

----- BASIS ----		2P
2P	1.160680	2.663909150886054E-001
2P	1.704720	5.231917972341583E-001
2P	3.039350	2.735309396155495E-001
2P	7.174820	1.292004438208935E-002

OXYGEN 1S(2)2S(2)2P(4), 3P

S-ORBITALS

----- BASIS ----		1S	2S
1S	7.61413	9.451499370424073E-001	-2.215694395858684E-001
1S	13.7574	3.390963896600367E-002	-4.759987960593645E-003
2S	1.69824	-3.399963800778900E-004	3.484391186952205E-001
2S	2.48022	2.409974341140337E-003	6.080684620164238E-001
2S	4.31196	-4.859948256407486E-003	2.536493584463399E-001
2S	5.86596	3.680960809019744E-002	-1.918295148068653E-001

P-ORBITALS

----- BASIS ----		2P
2P	1.14394	1.692205734038149E-001
2P	1.81730	5.797419644553105E-001
2P	3.44988	3.235210962510470E-001
2P	7.56484	1.660005624928098E-002

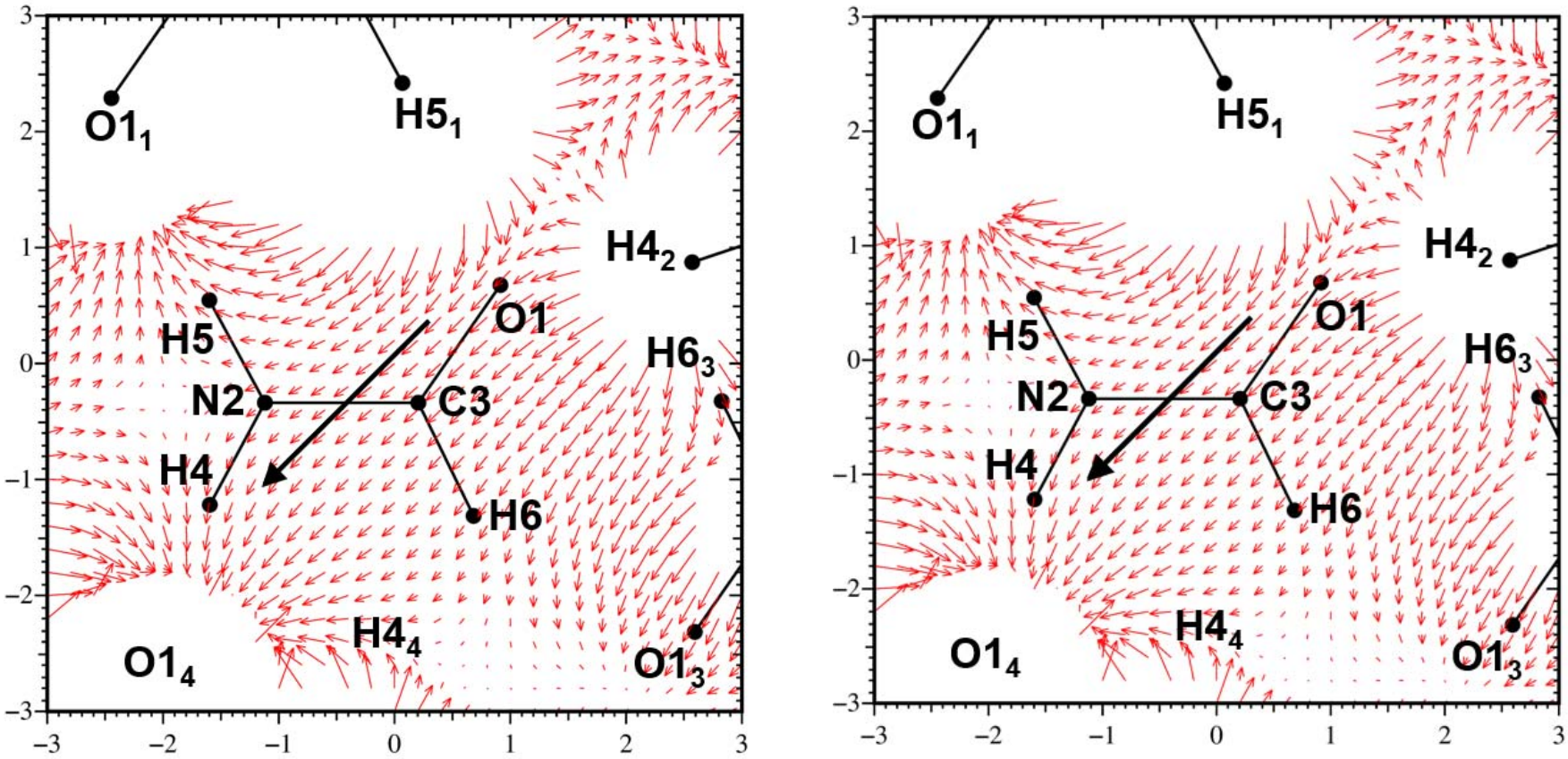
SULFUR K(2)L(8)3S(2)3P(4), 3P

S-ORBITALS

----- BASIS ----		1S	2S	3S
1S	16.01910	9.707644786471011E-001	-2.680778232090002E-001	7.777993133012676E-002
3S	19.45290	2.121987930909637E-002	-3.899968332270593E-003	2.439997845789525E-003
3S	13.77880	2.510985718432657E-002	4.868960464057825E-002	-2.130998118597327E-002
3S	9.85150	-2.869983676583722E-003	3.632270505976019E-001	-1.010699107680112E-001
3S	6.48374	1.939988966053108E-003	6.266249118078774E-001	-2.515797778867741E-001
3S	4.05540	-6.799961324309865E-004	5.413956038695639E-002	-6.276994458205267E-002
3S	2.67399	2.499985780996274E-004	-5.169958019958710E-003	6.510694251877813E-001
3S	1.66032	-6.999960186789566E-005	1.349989038093667E-003	5.017495570183993E-001

P-ORBITALS

----- BASIS ----		2P	2P
2P	8.00375	6.129347159581104E-001	-1.558583010984709E-001
4P	7.67346	-7.535935033543772E-001	-1.850159832711208E+001
4P	12.09980	3.667968378853311E-002	-1.198986930688224E-002
4P	7.67727	1.074140739952368E+000	1.839264951468632E+001
4P	5.32630	1.453787467060236E-001	9.040901451503114E-002
4P	2.87350	1.989982844579632E-003	5.269642559339228E-001
4P	1.67242	9.399918964346000E-004	4.946446082276314E-001
4P	1.03092	-1.399987930860042E-004	5.111944278297082E-002



a) ES **b)** DS ($-2 < x_f, y_f, z_f < 3$)

Figure S2 The comparison of EF maps in the plane of the formamide (FORM) molecule from the EP/MM-based **(a)** ES and **(b)** DS ($-2 < x_f, y_f, z_f < 3$) calculations. In both calculations, the R_{aMM} parameter was set to 9 Å.

Table S3 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central formamide (FORM) molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

Atom	Calculation	*XX*	*YY*	*ZZ*	*XY*	*XZ*	*YZ*
O1	Single molecule	-1304.611548	-1306.394319	-1306.434919	-0.301690	0.238592	-0.028909
	ES*	-0.006833	-0.003114	0.006161	0.000763	-0.003409	0.003929
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.006808	-0.003114	0.006136	0.000765	-0.003422	0.003929
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.006791	-0.003116	0.006121	0.000766	-0.003430	0.003928
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.006748	-0.003132	0.006094	0.000758	-0.003444	0.003921
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006705	-0.003246	0.006165	0.000615	-0.003539	0.003778
N2	Single molecule	-863.479007	-863.407391	-862.792412	0.033834	-0.161479	-0.264835
	ES*	0.002735	-0.001504	-0.001470	0.003925	0.002518	-0.000057
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002761	-0.001504	-0.001497	0.003928	0.002504	-0.000057
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002780	-0.001504	-0.001515	0.003929	0.002495	-0.000058
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002827	-0.001502	-0.001563	0.003926	0.002466	-0.000065
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003012	-0.001480	-0.001771	0.003934	0.002301	-0.000070
C3	Single molecule	-534.292168	-534.287130	-534.654728	-0.004788	0.112487	0.186057
	ES*	0.001081	-0.001546	0.000297	-0.000067	0.000551	-0.001043
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001107	-0.001547	0.000271	-0.000064	0.000539	-0.001043
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001124	-0.001547	0.000254	-0.000064	0.000532	-0.001044
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001167	-0.001550	0.000214	-0.000074	0.000514	-0.001056
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001267	-0.001473	0.000038	-0.000112	0.000381	-0.001148
H4	Single molecule	-1.905979	-2.375631	-1.914455	-0.122768	-0.062872	-0.227463
	ES*	-0.003159	0.001282	-0.003818	0.008083	0.003915	0.002837
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003132	0.001282	-0.003845	0.008086	0.003902	0.002837
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003113	0.001284	-0.003865	0.008087	0.003892	0.002837
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003065	0.001298	-0.003927	0.008095	0.003864	0.002830
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002856	0.001367	-0.004205	0.008246	0.003755	0.002850
H5	Single molecule	-2.381709	-1.888591	-1.875983	-0.119359	-0.173838	-0.054137
	ES*	0.009047	-0.010375	-0.004113	0.007462	0.004767	-0.000005
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.009073	-0.010376	-0.004139	0.007465	0.004753	-0.000005
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.009091	-0.010376	-0.004157	0.007466	0.004743	-0.000005
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.009139	-0.010384	-0.004197	0.007463	0.004715	-0.000009
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.009321	-0.010483	-0.004279	0.007394	0.004591	-0.000035
H6	Single molecule	-2.371888	-2.038319	-2.029989	-0.114117	-0.127805	-0.043414
	ES*	0.004028	-0.002041	-0.002590	-0.000762	-0.002143	-0.001567
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004053	-0.002041	-0.002615	-0.000760	-0.002154	-0.001567
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004070	-0.002041	-0.002632	-0.000760	-0.002159	-0.001569
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004105	-0.002028	-0.002679	-0.000777	-0.002169	-0.001593
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004221	-0.001976	-0.002834	-0.000700	-0.002171	-0.001526

Table S4 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **ABA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.53711	0.26451	0.12887	0.08684	0.30678
	ES*	0.12267	-0.01836	-0.01079	0.02524	0.03302
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.10784	-0.01835	-0.01079	0.02525	0.03302
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.10783	-0.01834	-0.01080	0.02525	0.03302
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.10780	-0.01832	-0.01081	0.02525	0.03302
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.10769	-0.01825	-0.01083	0.02527	0.03300
O2	Single molecule	-22.55797	0.03110	-0.08460	-0.28960	0.30331
	ES*	0.16613	-0.01373	0.01242	0.02070	0.02778
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.15136	-0.01372	0.01247	0.02071	0.02779
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.15138	-0.01372	0.01249	0.02071	0.02781
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.15145	-0.01371	0.01256	0.02072	0.02784
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.15172	-0.01367	0.01281	0.02074	0.02795
N1	Single molecule	-18.32641	-0.00848	-0.01346	-0.05028	0.05273
	ES*	-0.06416	0.00046	0.00171	0.01344	0.01355
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.07910	0.00051	0.00166	0.01346	0.01357
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.07918	0.00054	0.00163	0.01348	0.01359
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.07937	0.00062	0.00155	0.01352	0.01362
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.08030	0.00086	0.00130	0.01377	0.01386
C1	Single molecule	-14.81098	-0.00459	-0.00922	-0.06321	0.06404
	ES*	-0.01095	-0.00130	0.00274	0.02064	0.02086
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.02583	-0.00126	0.00272	0.02066	0.02088
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.02587	-0.00123	0.00271	0.02068	0.02089
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.02597	-0.00117	0.00267	0.02072	0.02093
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.02639	-0.00094	0.00254	0.02090	0.02107
C2	Single molecule	-14.82267	-0.00190	0.02170	0.00159	0.02184
	ES*	0.01486	-0.00013	-0.00229	0.01807	0.01821
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.00009	-0.00011	-0.00230	0.01807	0.01821
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.00011	-0.00009	-0.00231	0.01807	0.01821
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.00017	-0.00006	-0.00232	0.01807	0.01822
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.00035	0.00008	-0.00237	0.01809	0.01824
C3	Single molecule	-14.85963	-0.02080	-0.00574	-0.02883	0.03601
	ES*	0.05759	-0.00837	-0.00043	0.01553	0.01765
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04282	-0.00836	-0.00042	0.01553	0.01764
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04285	-0.00835	-0.00040	0.01553	0.01763
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04293	-0.00833	-0.00037	0.01553	0.01762
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04320	-0.00823	-0.00024	0.01553	0.01758

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C4	Single molecule	-14.83203	0.03847	0.00438	-0.03673	0.05337
	ES*	0.11255	-0.01316	0.00152	0.02094	0.02478
	DS* (-4 < x_f, y_f, z_f < 5)	0.09775	-0.01315	0.00154	0.02094	0.02478
	DS* (-3 < x_f, y_f, z_f < 4)	0.09776	-0.01314	0.00155	0.02094	0.02477
	DS* (-2 < x_f, y_f, z_f < 3)	0.09778	-0.01313	0.00158	0.02095	0.02477
	DS* (-1 < x_f, y_f, z_f < 2)	0.09785	-0.01307	0.00169	0.02096	0.02476
H1	Single molecule	-0.92249	0.04629	-0.00310	-0.03216	0.05645
	ES*	-0.09294	-0.02188	0.00016	0.01558	0.02686
	DS* (-4 < x_f, y_f, z_f < 5)	-0.10780	-0.02183	0.00011	0.01560	0.02683
	DS* (-3 < x_f, y_f, z_f < 4)	-0.10783	-0.02180	0.00007	0.01561	0.02681
	DS* (-2 < x_f, y_f, z_f < 3)	-0.10791	-0.02173	-0.00001	0.01564	0.02677
	DS* (-1 < x_f, y_f, z_f < 2)	-0.10861	-0.02145	-0.00032	0.01598	0.02676
H2	Single molecule	-0.92889	-0.01571	-0.02536	-0.01035	0.03158
	ES*	-0.08172	0.01480	0.01408	0.00111	0.02045
	DS* (-4 < x_f, y_f, z_f < 5)	-0.09662	0.01484	0.01401	0.00113	0.02044
	DS* (-3 < x_f, y_f, z_f < 4)	-0.09667	0.01487	0.01397	0.00114	0.02043
	DS* (-2 < x_f, y_f, z_f < 3)	-0.09679	0.01493	0.01387	0.00116	0.02041
	DS* (-1 < x_f, y_f, z_f < 2)	-0.09744	0.01514	0.01346	0.00135	0.02030
H3	Single molecule	-0.92455	-0.02749	0.02753	-0.03081	0.04962
	ES*	-0.08688	0.01209	-0.01343	0.01251	0.02198
	DS* (-4 < x_f, y_f, z_f < 5)	-0.10199	0.01215	-0.01349	0.01256	0.02208
	DS* (-3 < x_f, y_f, z_f < 4)	-0.10218	0.01219	-0.01353	0.01258	0.02214
	DS* (-2 < x_f, y_f, z_f < 3)	-0.10263	0.01229	-0.01363	0.01265	0.02228
	DS* (-1 < x_f, y_f, z_f < 2)	-0.10436	0.01264	-0.01370	0.01288	0.02266
H4	Single molecule	-1.12384	-0.00480	0.00456	-0.01685	0.01811
	ES*	0.01602	-0.00566	0.00401	0.02285	0.02388
	DS* (-4 < x_f, y_f, z_f < 5)	0.00109	-0.00561	0.00399	0.02289	0.02390
	DS* (-3 < x_f, y_f, z_f < 4)	0.00101	-0.00558	0.00397	0.02291	0.02391
	DS* (-2 < x_f, y_f, z_f < 3)	0.00083	-0.00552	0.00393	0.02296	0.02394
	DS* (-1 < x_f, y_f, z_f < 2)	0.00011	-0.00528	0.00379	0.02317	0.02406
H5	Single molecule	-1.09164	0.00931	0.00820	-0.01511	0.01955
	ES*	-0.00844	-0.00259	0.00272	0.01608	0.01652
	DS* (-4 < x_f, y_f, z_f < 5)	-0.02330	-0.00255	0.00271	0.01612	0.01654
	DS* (-3 < x_f, y_f, z_f < 4)	-0.02333	-0.00251	0.00270	0.01615	0.01656
	DS* (-2 < x_f, y_f, z_f < 3)	-0.02341	-0.00244	0.00268	0.01621	0.01661
	DS* (-1 < x_f, y_f, z_f < 2)	-0.02374	-0.00216	0.00261	0.01645	0.01679
H6	Single molecule	-1.12410	0.00241	-0.00010	-0.02469	0.02481
	ES*	0.01505	0.00364	-0.00511	0.02153	0.02243
	DS* (-4 < x_f, y_f, z_f < 5)	0.00028	0.00365	-0.00513	0.02152	0.02243
	DS* (-3 < x_f, y_f, z_f < 4)	0.00032	0.00366	-0.00515	0.02152	0.02242
	DS* (-2 < x_f, y_f, z_f < 3)	0.00040	0.00369	-0.00519	0.02150	0.02242
	DS* (-1 < x_f, y_f, z_f < 2)	0.00065	0.00376	-0.00532	0.02144	0.02241

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H7	Single molecule	-1.09866	0.00748	0.00249	-0.02136	0.02277
	ES*	0.00318	0.00419	-0.00467	0.01755	0.01864
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01155	0.00422	-0.00468	0.01754	0.01864
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01150	0.00423	-0.00468	0.01754	0.01864
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01137	0.00426	-0.00469	0.01753	0.01864
	DS* (-1 < x_f, y_f, z_f < 2)	-0.01092	0.00441	-0.00473	0.01751	0.01866
H8	Single molecule	-1.15807	0.00928	-0.00939	-0.00454	0.01396
	ES*	0.05209	-0.00967	0.00537	0.00661	0.01289
	DS* (-4 < x_f, y_f, z_f < 5)	0.03729	-0.00967	0.00540	0.00659	0.01289
	DS* (-3 < x_f, y_f, z_f < 4)	0.03730	-0.00967	0.00542	0.00658	0.01289
	DS* (-2 < x_f, y_f, z_f < 3)	0.03733	-0.00966	0.00547	0.00655	0.01289
	DS* (-1 < x_f, y_f, z_f < 2)	0.03741	-0.00966	0.00568	0.00643	0.01292
H9	Single molecule	-1.15042	0.01203	0.00773	-0.01026	0.01760
	ES*	0.04967	-0.01151	-0.00715	0.01738	0.02203
	DS* (-4 < x_f, y_f, z_f < 5)	0.03497	-0.01149	-0.00712	0.01739	0.02202
	DS* (-3 < x_f, y_f, z_f < 4)	0.03504	-0.01147	-0.00710	0.01740	0.02201
	DS* (-2 < x_f, y_f, z_f < 3)	0.03521	-0.01144	-0.00704	0.01742	0.02199
	DS* (-1 < x_f, y_f, z_f < 2)	0.03592	-0.01127	-0.00683	0.01751	0.02192

Table S5 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ABA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.220117	-1306.380383	-1305.246796	-0.187214	-0.702478	0.113783
	ES*	-0.002550	-0.005923	0.005038	-0.010777	0.003706	0.001193
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002548	-0.005927	0.005040	-0.010783	0.003710	0.001184
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002547	-0.005929	0.005042	-0.010786	0.003713	0.001178
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002544	-0.005935	0.005045	-0.010795	0.003719	0.001164
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002534	-0.005957	0.005056	-0.010831	0.003740	0.001112
O2	Single molecule	-1305.012168	-1306.234388	-1306.578111	0.440122	-0.136701	-0.125524
	ES*	-0.017714	0.001048	0.008959	-0.012626	0.001168	-0.006716
	DS* (-4 < x_f, y_f, z_f < 5)	-0.017712	0.001044	0.008961	-0.012631	0.001172	-0.006724
	DS* (-3 < x_f, y_f, z_f < 4)	-0.017711	0.001042	0.008963	-0.012635	0.001175	-0.006730
	DS* (-2 < x_f, y_f, z_f < 3)	-0.017708	0.001035	0.008966	-0.012644	0.001181	-0.006744
	DS* (-1 < x_f, y_f, z_f < 2)	-0.017699	0.001013	0.008980	-0.012683	0.001204	-0.006797
N1	Single molecule	-863.498495	-863.492994	-863.400031	-0.001310	0.013967	0.027164
	ES*	0.004809	0.001139	-0.006443	0.000379	-0.002018	-0.002903
	DS* (-4 < x_f, y_f, z_f < 5)	0.004811	0.001135	-0.006442	0.000374	-0.002014	-0.002912
	DS* (-3 < x_f, y_f, z_f < 4)	0.004812	0.001133	-0.006441	0.000370	-0.002012	-0.002917
	DS* (-2 < x_f, y_f, z_f < 3)	0.004815	0.001128	-0.006439	0.000362	-0.002007	-0.002931
	DS* (-1 < x_f, y_f, z_f < 2)	0.004830	0.001043	-0.006368	0.000342	-0.002001	-0.002946
C1	Single molecule	-533.901156	-533.898839	-534.221168	-0.028335	-0.057896	-0.090993
	ES*	-0.000362	-0.000106	0.000401	0.001395	0.001568	0.001059
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000360	-0.000110	0.000403	0.001390	0.001572	0.001050
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000359	-0.000112	0.000404	0.001386	0.001574	0.001044
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000356	-0.000117	0.000406	0.001377	0.001580	0.001030
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000350	-0.000139	0.000423	0.001347	0.001594	0.000988
C2	Single molecule	-533.808143	-533.841907	-533.868032	0.025323	-0.012059	-0.011662
	ES*	-0.000611	-0.001195	0.001727	0.001148	0.002519	-0.000108
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000609	-0.001198	0.001729	0.001142	0.002523	-0.000117
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000608	-0.001201	0.001730	0.001138	0.002525	-0.000122
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000606	-0.001206	0.001733	0.001129	0.002531	-0.000136
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000602	-0.001227	0.001750	0.001092	0.002554	-0.000192
C3	Single molecule	-533.862834	-533.800716	-533.873838	-0.016610	0.005268	-0.011363
	ES*	-0.000787	0.001550	-0.000840	0.000186	0.002976	-0.002047
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000785	0.001546	-0.000838	0.000181	0.002980	-0.002055
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000784	0.001543	-0.000836	0.000177	0.002983	-0.002061
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000781	0.001537	-0.000833	0.000168	0.002989	-0.002075
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000776	0.001518	-0.000819	0.000126	0.003011	-0.002131

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C4	Single molecule	-534.039845	-534.333910	-533.927325	0.161939	0.033343	0.195150
	ES*	-0.001164	0.000912	-0.000122	-0.002352	0.001987	-0.003226
	DS* (-4 < x_f, y_f, z_f < 5)	-0.001162	0.000908	-0.000120	-0.002358	0.001991	-0.003234
	DS* (-3 < x_f, y_f, z_f < 4)	-0.001161	0.000906	-0.000119	-0.002361	0.001993	-0.003240
	DS* (-2 < x_f, y_f, z_f < 3)	-0.001158	0.000900	-0.000116	-0.002370	0.002000	-0.003254
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001149	0.000878	-0.000103	-0.002409	0.002022	-0.003308
H1	Single molecule	-2.103167	-1.816018	-1.887151	0.051957	0.154601	-0.026980
	ES*	0.011399	-0.013768	-0.012880	-0.000756	-0.007259	0.000027
	DS* (-4 < x_f, y_f, z_f < 5)	0.011401	-0.013772	-0.012878	-0.000762	-0.007255	0.000019
	DS* (-3 < x_f, y_f, z_f < 4)	0.011402	-0.013774	-0.012877	-0.000765	-0.007253	0.000013
	DS* (-2 < x_f, y_f, z_f < 3)	0.011405	-0.013778	-0.012875	-0.000774	-0.007248	0.000000
	DS* (-1 < x_f, y_f, z_f < 2)	0.011339	-0.013876	-0.012712	-0.000757	-0.007233	-0.000065
H2	Single molecule	-1.939294	-2.115067	-1.797704	-0.207783	-0.006053	-0.006717
	ES*	-0.000407	0.002171	-0.014371	0.012262	-0.004606	-0.007338
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000405	0.002167	-0.014369	0.012257	-0.004602	-0.007347
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000404	0.002165	-0.014368	0.012253	-0.004600	-0.007352
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000400	0.002160	-0.014366	0.012244	-0.004595	-0.007365
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000399	0.002096	-0.014304	0.012211	-0.004578	-0.007448
H3	Single molecule	-1.907764	-2.019269	-1.893098	0.147364	-0.095786	0.138766
	ES*	-0.002685	0.002567	-0.016023	-0.010544	0.004364	-0.005799
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002683	0.002563	-0.016021	-0.010550	0.004367	-0.005808
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002682	0.002561	-0.016021	-0.010554	0.004370	-0.005813
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002679	0.002557	-0.016020	-0.010562	0.004375	-0.005826
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002574	0.002456	-0.016022	-0.010610	0.004416	-0.005673
H4	Single molecule	-2.295756	-1.958828	-2.051774	0.052522	0.153894	-0.033804
	ES*	-0.002133	0.000946	0.001053	0.001148	0.001219	0.001982
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002131	0.000942	0.001055	0.001142	0.001223	0.001973
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002130	0.000940	0.001056	0.001138	0.001225	0.001968
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002127	0.000935	0.001058	0.001130	0.001231	0.001953
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002117	0.000916	0.001068	0.001094	0.001249	0.001908
H5	Single molecule	-2.055331	-2.276438	-1.975704	-0.183922	-0.002093	0.001965
	ES*	-0.000894	-0.001072	0.001216	0.001757	0.002598	0.001534
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000892	-0.001075	0.001218	0.001752	0.002601	0.001525
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000891	-0.001078	0.001219	0.001748	0.002604	0.001519
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000888	-0.001082	0.001221	0.001739	0.002609	0.001505
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000884	-0.001091	0.001227	0.001712	0.002613	0.001461
H6	Single molecule	-2.048907	-2.286439	-1.968377	-0.180686	-0.031549	-0.037560
	ES*	0.002013	-0.003947	0.001187	0.001253	0.005238	-0.000193
	DS* (-4 < x_f, y_f, z_f < 5)	0.002014	-0.003951	0.001189	0.001247	0.005242	-0.000202
	DS* (-3 < x_f, y_f, z_f < 4)	0.002016	-0.003954	0.001190	0.001243	0.005244	-0.000208
	DS* (-2 < x_f, y_f, z_f < 3)	0.002018	-0.003959	0.001193	0.001234	0.005250	-0.000221
	DS* (-1 < x_f, y_f, z_f < 2)	0.002026	-0.003982	0.001209	0.001197	0.005272	-0.000277

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-2.294049	-1.957587	-2.044386	0.034695	0.159819	-0.013993
	ES*	-0.002058	-0.003041	0.004817	0.000444	0.001399	-0.001155
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002056	-0.003045	0.004819	0.000439	0.001402	-0.001164
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002055	-0.003047	0.004820	0.000435	0.001405	-0.001169
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002053	-0.003053	0.004823	0.000426	0.001410	-0.001183
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002049	-0.003069	0.004835	0.000384	0.001440	-0.001242
H8	Single molecule	-2.160270	-2.111476	-2.029731	0.178526	-0.116605	0.102861
	ES*	-0.003048	0.002748	-0.000376	-0.001239	0.004427	-0.004888
	DS* (-4 < x_f, y_f, z_f < 5)	-0.003046	0.002744	-0.000374	-0.001245	0.004431	-0.004896
	DS* (-3 < x_f, y_f, z_f < 4)	-0.003045	0.002741	-0.000373	-0.001248	0.004434	-0.004902
	DS* (-2 < x_f, y_f, z_f < 3)	-0.003043	0.002736	-0.000369	-0.001257	0.004440	-0.004916
	DS* (-1 < x_f, y_f, z_f < 2)	-0.003032	0.002710	-0.000355	-0.001306	0.004467	-0.004973
H9	Single molecule	-2.004473	-2.327922	-1.966912	-0.137002	-0.017615	-0.051469
	ES*	-0.000634	0.005177	-0.005142	0.003178	0.003314	-0.001114
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000633	0.005173	-0.005140	0.003172	0.003318	-0.001123
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000631	0.005170	-0.005138	0.003168	0.003320	-0.001129
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000629	0.005164	-0.005135	0.003159	0.003326	-0.001143
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000630	0.005151	-0.005120	0.003118	0.003347	-0.001201

Table S6 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ABA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-0.406528	-0.646926	1.053453	-0.280821	-1.053717	0.170674
	ES*	-0.002108	-0.007167	0.009275	-0.016166	0.005559	0.001789
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002105	-0.007173	0.009278	-0.016174	0.005565	0.001776
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002104	-0.007176	0.009280	-0.016180	0.005569	0.001767
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002099	-0.007185	0.009284	-0.016193	0.005578	0.001747
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002083	-0.007219	0.009302	-0.016246	0.005610	0.001667
O2	Single molecule	1.394082	-0.439248	-0.954833	0.660183	-0.205051	-0.188286
	ES*	-0.022717	0.005425	0.017292	-0.018938	0.001753	-0.010073
	DS* (-4 < x_f, y_f, z_f < 5)	-0.022714	0.005419	0.017295	-0.018947	0.001758	-0.010086
	DS* (-3 < x_f, y_f, z_f < 4)	-0.022713	0.005416	0.017297	-0.018952	0.001762	-0.010095
	DS* (-2 < x_f, y_f, z_f < 3)	-0.022709	0.005406	0.017303	-0.018966	0.001772	-0.010116
	DS* (-1 < x_f, y_f, z_f < 2)	-0.022696	0.005373	0.017323	-0.019025	0.001806	-0.010196
N1	Single molecule	-0.051983	-0.043730	0.095713	-0.001965	0.020951	0.040747
	ES*	0.007462	0.001956	-0.009417	0.000569	-0.003027	-0.004355
	DS* (-4 < x_f, y_f, z_f < 5)	0.007465	0.001950	-0.009415	0.000561	-0.003021	-0.004368
	DS* (-3 < x_f, y_f, z_f < 4)	0.007466	0.001947	-0.009413	0.000555	-0.003018	-0.004376
	DS* (-2 < x_f, y_f, z_f < 3)	0.007471	0.001940	-0.009411	0.000542	-0.003010	-0.004396
	DS* (-1 < x_f, y_f, z_f < 2)	0.007492	0.001812	-0.009304	0.000514	-0.003001	-0.004419
C1	Single molecule	0.158848	0.162323	-0.321171	-0.042503	-0.086843	-0.136490
	ES*	-0.000510	-0.000126	0.000635	0.002093	0.002352	0.001588
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000507	-0.000131	0.000638	0.002084	0.002358	0.001575
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000505	-0.000135	0.000640	0.002079	0.002361	0.001566
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000501	-0.000142	0.000643	0.002066	0.002370	0.001545
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000492	-0.000176	0.000668	0.002021	0.002390	0.001482
C2	Single molecule	0.046827	-0.003820	-0.043007	0.037984	-0.018089	-0.017493
	ES*	-0.000877	-0.001752	0.002630	0.001721	0.003779	-0.000162
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000875	-0.001758	0.002633	0.001713	0.003784	-0.000175
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000873	-0.001762	0.002635	0.001707	0.003788	-0.000183
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000869	-0.001770	0.002639	0.001694	0.003797	-0.000204
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000863	-0.001801	0.002664	0.001638	0.003831	-0.000288

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C3	Single molecule	-0.025557	0.067620	-0.042063	-0.024915	0.007902	-0.017045
	ES*	-0.001142	0.002363	-0.001221	0.000280	0.004464	-0.003070
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001139	0.002357	-0.001218	0.000271	0.004470	-0.003083
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001137	0.002353	-0.001216	0.000266	0.004474	-0.003092
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001134	0.002345	-0.001211	0.000252	0.004483	-0.003113
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001125	0.002315	-0.001190	0.000189	0.004517	-0.003197
C4	Single molecule	0.090773	-0.350325	0.259553	0.242908	0.050015	0.292726
	ES*	-0.001559	0.001555	0.000004	-0.003528	0.002980	-0.004838
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001556	0.001549	0.000007	-0.003537	0.002986	-0.004852
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001554	0.001546	0.000009	-0.003542	0.002990	-0.004860
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001550	0.001537	0.000014	-0.003555	0.002999	-0.004881
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001536	0.001504	0.000033	-0.003613	0.003033	-0.004962
H1	Single molecule	-0.251582	0.179141	0.072441	0.077935	0.231901	-0.040470
	ES*	0.024723	-0.013028	-0.011695	-0.001134	-0.010889	0.000041
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.024726	-0.013033	-0.011693	-0.001143	-0.010883	0.000028
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.024728	-0.013036	-0.011691	-0.001148	-0.010880	0.000020
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.024732	-0.013043	-0.011689	-0.001161	-0.010872	0.000000
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.024633	-0.013189	-0.011444	-0.001135	-0.010850	-0.000098
H2	Single molecule	0.017091	-0.246568	0.229477	-0.311675	-0.009079	-0.010075
	ES*	0.005693	0.009560	-0.015253	0.018393	-0.006909	-0.011008
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005696	0.009554	-0.015250	0.018385	-0.006904	-0.011021
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005698	0.009551	-0.015249	0.018380	-0.006900	-0.011029
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005703	0.009543	-0.015246	0.018367	-0.006892	-0.011048
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005705	0.009448	-0.015153	0.018316	-0.006868	-0.011172
H3	Single molecule	0.048420	-0.118838	0.070418	0.221047	-0.143679	0.208149
	ES*	0.004043	0.011921	-0.015964	-0.015817	0.006546	-0.008698
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004046	0.011916	-0.015961	-0.015825	0.006551	-0.008711
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004048	0.011913	-0.015960	-0.015830	0.006555	-0.008720
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004052	0.011907	-0.015959	-0.015843	0.006562	-0.008740
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004209	0.011754	-0.015962	-0.015915	0.006624	-0.008509
H4	Single molecule	-0.290455	0.214936	0.075518	0.078783	0.230841	-0.050705
	ES*	-0.003132	0.001486	0.001646	0.001722	0.001829	0.002973
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003129	0.001480	0.001649	0.001713	0.001835	0.002960
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003127	0.001477	0.001650	0.001708	0.001838	0.002951
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003123	0.001469	0.001654	0.001694	0.001847	0.002930
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003109	0.001441	0.001668	0.001642	0.001873	0.002862

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H5	Single molecule	0.070740	-0.260921	0.190181	-0.275882	-0.003140	0.002948
	ES*	-0.000966	-0.001233	0.002199	0.002636	0.003896	0.002301
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000963	-0.001239	0.002202	0.002627	0.003902	0.002288
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000961	-0.001242	0.002203	0.002622	0.003906	0.002279
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000957	-0.001249	0.002206	0.002609	0.003914	0.002257
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000952	-0.001263	0.002214	0.002568	0.003919	0.002192
H6	Single molecule	0.078501	-0.277797	0.199296	-0.271030	-0.047323	-0.056340
	ES*	0.003393	-0.005547	0.002154	0.001879	0.007857	-0.000290
	DS* (-4 < x_f, y_f, z_f < 5)	0.003396	-0.005553	0.002157	0.001870	0.007863	-0.000303
	DS* (-3 < x_f, y_f, z_f < 4)	0.003397	-0.005557	0.002159	0.001865	0.007866	-0.000311
	DS* (-2 < x_f, y_f, z_f < 3)	0.003402	-0.005565	0.002164	0.001851	0.007875	-0.000332
	DS* (-1 < x_f, y_f, z_f < 2)	0.003413	-0.005600	0.002187	0.001796	0.007909	-0.000415
H7	Single molecule	-0.293063	0.211631	0.081432	0.052043	0.239729	-0.020989
	ES*	-0.002946	-0.004420	0.007366	0.000666	0.002098	-0.001732
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002943	-0.004426	0.007369	0.000658	0.002104	-0.001745
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002942	-0.004430	0.007371	0.000653	0.002107	-0.001754
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002938	-0.004438	0.007376	0.000639	0.002115	-0.001774
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002932	-0.004462	0.007394	0.000577	0.002160	-0.001864
H8	Single molecule	-0.089667	-0.016476	0.106142	0.267789	-0.174908	0.154291
	ES*	-0.004234	0.004460	-0.000226	-0.001858	0.006641	-0.007331
	DS* (-4 < x_f, y_f, z_f < 5)	-0.004231	0.004454	-0.000223	-0.001867	0.006647	-0.007344
	DS* (-3 < x_f, y_f, z_f < 4)	-0.004230	0.004450	-0.000221	-0.001872	0.006650	-0.007353
	DS* (-2 < x_f, y_f, z_f < 3)	-0.004226	0.004441	-0.000215	-0.001886	0.006659	-0.007374
	DS* (-1 < x_f, y_f, z_f < 2)	-0.004210	0.004403	-0.000194	-0.001959	0.006700	-0.007460
H9	Single molecule	0.142943	-0.342230	0.199286	-0.205503	-0.026422	-0.077204
	ES*	-0.000652	0.008065	-0.007413	0.004766	0.004971	-0.001671
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000649	0.008059	-0.007410	0.004758	0.004977	-0.001685
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000648	0.008055	-0.007408	0.004752	0.004981	-0.001693
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000644	0.008046	-0.007402	0.004739	0.004990	-0.001715
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000646	0.008026	-0.007380	0.004677	0.005021	-0.001802

Table S7 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **ACG** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.36458	0.08173	-0.28854	-0.08212	0.31093
	ES*	0.02511	-0.00444	0.00477	0.00564	0.00862
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01947	-0.00441	0.00479	0.00564	0.00862
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01960	-0.00438	0.00481	0.00565	0.00861
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02015	-0.00423	0.00480	0.00566	0.00854
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02535	-0.00269	0.00423	0.00597	0.00780
O2	Single molecule	-22.38763	-0.11167	0.29727	0.11082	0.33633
	ES*	0.03775	0.00352	-0.00964	-0.00603	0.01190
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.03200	0.00354	-0.00961	-0.00602	0.01187
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.03205	0.00355	-0.00958	-0.00601	0.01185
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.03236	0.00364	-0.00947	-0.00598	0.01178
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.03614	0.00484	-0.00837	-0.00568	0.01121
O3	Single molecule	-22.41714	0.16019	-0.27385	-0.11299	0.33678
	ES*	0.07465	-0.02355	0.00541	0.02093	0.03197
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06874	-0.02351	0.00538	0.02092	0.03193
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06866	-0.02348	0.00536	0.02092	0.03190
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06846	-0.02337	0.00532	0.02091	0.03181
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06751	-0.02261	0.00515	0.02090	0.03122
N4	Single molecule	-18.40748	-0.00493	-0.00450	0.00424	0.00791
	ES*	0.01638	-0.00157	0.00779	0.00227	0.00826
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01059	-0.00154	0.00779	0.00227	0.00826
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01059	-0.00153	0.00779	0.00227	0.00826
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01067	-0.00145	0.00781	0.00228	0.00827
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01160	-0.00085	0.00811	0.00232	0.00848
C5	Single molecule	-14.72083	0.02795	0.04414	-0.02457	0.05773
	ES*	0.02579	-0.00023	-0.00058	-0.00065	0.00090
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02008	-0.00020	-0.00056	-0.00064	0.00088
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02015	-0.00018	-0.00055	-0.00064	0.00086
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02055	-0.00005	-0.00050	-0.00062	0.00080
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02488	0.00142	-0.00021	-0.00038	0.00148
C6	Single molecule	-14.80420	-0.02783	-0.04321	0.02640	0.05778
	ES*	0.02727	-0.00184	0.00424	0.00111	0.00475
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02151	-0.00181	0.00424	0.00111	0.00474
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02153	-0.00178	0.00424	0.00111	0.00473
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02172	-0.00167	0.00425	0.00111	0.00470
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02381	-0.00065	0.00433	0.00118	0.00454

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C7	Single molecule	-14.73410	0.02852	-0.01503	-0.02292	0.03955
	ES*	0.03136	-0.00777	0.00974	0.00765	0.01462
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02553	-0.00774	0.00973	0.00765	0.01459
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02550	-0.00772	0.00972	0.00765	0.01458
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02546	-0.00765	0.00970	0.00765	0.01453
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02540	-0.00714	0.00969	0.00766	0.01427
C8	Single molecule	-14.82079	0.00947	0.00769	0.00566	0.01344
	ES*	0.01664	-0.00506	0.00851	0.00658	0.01189
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01084	-0.00505	0.00849	0.00659	0.01188
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01083	-0.00503	0.00848	0.00659	0.01187
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01081	-0.00501	0.00846	0.00660	0.01184
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01069	-0.00496	0.00835	0.00661	0.01175
H9	Single molecule	-1.09288	0.00069	-0.00015	-0.01337	0.01339
	ES*	0.02989	-0.00510	0.00376	-0.00091	0.00640
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02415	-0.00505	0.00377	-0.00091	0.00637
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02421	-0.00502	0.00377	-0.00090	0.00634
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02449	-0.00488	0.00376	-0.00089	0.00622
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02746	-0.00366	0.00361	-0.00082	0.00520
H10	Single molecule	-1.09086	0.02046	0.00106	0.00526	0.02115
	ES*	0.03232	-0.00111	0.00563	0.00449	0.00729
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02651	-0.00108	0.00563	0.00448	0.00727
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02650	-0.00105	0.00562	0.00447	0.00726
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02652	-0.00095	0.00561	0.00446	0.00723
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02717	-0.00012	0.00553	0.00447	0.00711
H11	Single molecule	-1.01573	-0.00851	-0.01017	0.00861	0.01581
	ES*	-0.00272	0.00090	0.01708	0.00066	0.01712
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.00851	0.00091	0.01709	0.00067	0.01713
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.00850	0.00092	0.01710	0.00067	0.01714
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.00845	0.00095	0.01715	0.00069	0.01719
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.00786	0.00126	0.01774	0.00072	0.01780
H12	Single molecule	-1.00950	0.06416	-0.01972	-0.05965	0.08980
	ES*	-0.00750	-0.01791	0.00664	0.01801	0.02625
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.01309	-0.01787	0.00667	0.01801	0.02624
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.01293	-0.01784	0.00669	0.01801	0.02622
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.01216	-0.01766	0.00669	0.01804	0.02612
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.00502	-0.01591	0.00602	0.01849	0.02513
H13	Single molecule	-1.03361	-0.05434	0.02561	-0.16663	0.17713
	ES*	0.02086	-0.00581	0.00724	0.00426	0.01021
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01508	-0.00579	0.00722	0.00427	0.01019
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01509	-0.00577	0.00721	0.00428	0.01018
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01512	-0.00574	0.00719	0.00429	0.01015
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01507	-0.00570	0.00720	0.00433	0.01015

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H14	Single molecule	-1.05780	0.11610	0.01677	0.00648	0.11748
	ES*	0.02480	-0.00207	0.00605	0.00565	0.00853
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01897	-0.00206	0.00602	0.00565	0.00851
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01894	-0.00205	0.00600	0.00565	0.00849
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01888	-0.00203	0.00594	0.00565	0.00844
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01871	-0.00199	0.00546	0.00560	0.00808
H15	Single molecule	-1.06152	-0.02145	0.046251	0.03342	0.060961
	ES*	-0.00743	-0.00672	0.008476	0.008332	0.013655
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.01322	-0.00672	0.008469	0.008343	0.013655
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.01321	-0.00672	0.008465	0.008349	0.013656
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.01322	-0.00673	0.008459	0.008363	0.013666
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.01336	-0.00698	0.008484	0.008374	0.013815

Table S8 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ACG** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.414782	-1306.205327	-1306.250919	-0.447312	0.911156	0.395135
	ES*	0.001547	-0.004076	0.001828	-0.000960	-0.004397	-0.000080
	DS* (-4 < x_f, y_f, z_f < 5)	0.001547	-0.004074	0.001827	-0.000965	-0.004400	-0.000077
	DS* (-3 < x_f, y_f, z_f < 4)	0.001545	-0.004071	0.001826	-0.000968	-0.004403	-0.000075
	DS* (-2 < x_f, y_f, z_f < 3)	0.001521	-0.004044	0.001824	-0.000964	-0.004411	-0.000070
	DS* (-1 < x_f, y_f, z_f < 2)	0.001183	-0.003678	0.001796	-0.000740	-0.004584	0.000009
O2	Single molecule	-1305.631482	-1305.874421	-1305.790640	0.575824	-0.836566	-0.516193
	ES*	0.002314	-0.004415	0.000793	0.004711	-0.000426	-0.004658
	DS* (-4 < x_f, y_f, z_f < 5)	0.002314	-0.004413	0.000791	0.004705	-0.000429	-0.004655
	DS* (-3 < x_f, y_f, z_f < 4)	0.002312	-0.004410	0.000790	0.004700	-0.000432	-0.004654
	DS* (-2 < x_f, y_f, z_f < 3)	0.002292	-0.004388	0.000789	0.004671	-0.000439	-0.004653
	DS* (-1 < x_f, y_f, z_f < 2)	0.001989	-0.004101	0.000805	0.004335	-0.000581	-0.004716
O3	Single molecule	-1305.768987	-1305.834135	-1305.759655	0.624008	-0.587797	-0.613249
	ES*	-0.012046	0.010563	-0.007263	-0.000750	0.018454	0.001886
	DS* (-4 < x_f, y_f, z_f < 5)	-0.012046	0.010565	-0.007264	-0.000756	0.018451	0.001888
	DS* (-3 < x_f, y_f, z_f < 4)	-0.012046	0.010566	-0.007265	-0.000760	0.018448	0.001890
	DS* (-2 < x_f, y_f, z_f < 3)	-0.012046	0.010568	-0.007267	-0.000773	0.018443	0.001893
	DS* (-1 < x_f, y_f, z_f < 2)	-0.012034	0.010559	-0.007271	-0.000863	0.018422	0.001897
N4	Single molecule	-863.035898	-863.300891	-862.957943	0.062377	0.345561	-0.014109
	ES*	-0.001454	0.002425	-0.001063	0.000504	0.001745	0.000264
	DS* (-4 < x_f, y_f, z_f < 5)	-0.001454	0.002427	-0.001065	0.000499	0.001742	0.000266
	DS* (-3 < x_f, y_f, z_f < 4)	-0.001455	0.002428	-0.001066	0.000494	0.001739	0.000268
	DS* (-2 < x_f, y_f, z_f < 3)	-0.001460	0.002436	-0.001068	0.000475	0.001733	0.000271
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001545	0.002521	-0.001069	0.000288	0.001719	0.000265
C5	Single molecule	-534.443124	-534.251551	-534.489407	-0.072044	-0.319053	0.079495
	ES*	0.001107	-0.002054	0.000803	0.001363	-0.000277	-0.002048
	DS* (-4 < x_f, y_f, z_f < 5)	0.001106	-0.002052	0.000801	0.001357	-0.000280	-0.002046
	DS* (-3 < x_f, y_f, z_f < 4)	0.001105	-0.002050	0.000800	0.001353	-0.000283	-0.002044
	DS* (-2 < x_f, y_f, z_f < 3)	0.001083	-0.002026	0.000798	0.001340	-0.000291	-0.002041
	DS* (-1 < x_f, y_f, z_f < 2)	0.000701	-0.001676	0.000831	0.001251	-0.000417	-0.002044
C6	Single molecule	-533.515496	-533.701994	-533.517811	-0.053590	0.028970	0.063635
	ES*	0.000021	-0.000388	0.000312	0.000905	0.001753	-0.000424
	DS* (-4 < x_f, y_f, z_f < 5)	0.000020	-0.000386	0.000311	0.000899	0.001750	-0.000421
	DS* (-3 < x_f, y_f, z_f < 4)	0.000020	-0.000385	0.000310	0.000895	0.001747	-0.000420
	DS* (-2 < x_f, y_f, z_f < 3)	0.000008	-0.000371	0.000308	0.000884	0.001741	-0.000416
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000176	-0.000196	0.000317	0.000826	0.001711	-0.000412

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C7	Single molecule	-534.642194	-534.427719	-534.711607	-0.092067	-0.242834	0.027954
	ES*	-0.000773	0.000587	-0.000070	0.002045	0.003392	-0.000990
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000774	0.000589	-0.000072	0.002039	0.003388	-0.000987
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000774	0.000590	-0.000073	0.002035	0.003386	-0.000985
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000776	0.000594	-0.000075	0.002017	0.003380	-0.000983
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000793	0.000619	-0.000082	0.001853	0.003360	-0.000984
C8	Single molecule	-533.292116	-533.249100	-533.317107	0.008844	0.000472	0.001506
	ES*	0.000720	-0.001809	0.001026	0.000037	-0.000015	0.000484
	DS* (-4 < x_f, y_f, z_f < 5)	0.000720	-0.001807	0.001025	0.000032	-0.000018	0.000487
	DS* (-3 < x_f, y_f, z_f < 4)	0.000719	-0.001806	0.001024	0.000027	-0.000021	0.000488
	DS* (-2 < x_f, y_f, z_f < 3)	0.000719	-0.001803	0.001021	0.000007	-0.000027	0.000491
	DS* (-1 < x_f, y_f, z_f < 2)	0.000724	-0.001799	0.001012	-0.000186	-0.000050	0.000492
H9	Single molecule	-1.934816	-2.027644	-2.154166	-0.095752	-0.123800	-0.190926
	ES*	0.000005	-0.000476	0.000110	0.000432	0.001172	0.001640
	DS* (-4 < x_f, y_f, z_f < 5)	0.000004	-0.000474	0.000108	0.000426	0.001168	0.001643
	DS* (-3 < x_f, y_f, z_f < 4)	0.000003	-0.000472	0.000107	0.000423	0.001166	0.001645
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000012	-0.000454	0.000104	0.000417	0.001159	0.001649
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000239	-0.000221	0.000098	0.000449	0.001143	0.001652
H10	Single molecule	-2.157253	-2.003541	-1.962310	0.178442	-0.156305	0.109349
	ES*	0.000064	-0.001341	0.000779	-0.000175	0.000952	-0.000070
	DS* (-4 < x_f, y_f, z_f < 5)	0.000064	-0.001340	0.000778	-0.000181	0.000949	-0.000067
	DS* (-3 < x_f, y_f, z_f < 4)	0.000063	-0.001338	0.000777	-0.000184	0.000947	-0.000066
	DS* (-2 < x_f, y_f, z_f < 3)	0.000058	-0.001331	0.000774	-0.000191	0.000940	-0.000061
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000015	-0.001255	0.000771	-0.000192	0.000911	-0.000046
H11	Single molecule	-1.958532	-2.278459	-1.925448	0.202796	0.119334	-0.170812
	ES*	-0.005270	0.008819	-0.006126	-0.001326	0.000533	0.001561
	DS* (-4 < x_f, y_f, z_f < 5)	-0.005270	0.008821	-0.006127	-0.001332	0.000530	0.001564
	DS* (-3 < x_f, y_f, z_f < 4)	-0.005270	0.008822	-0.006128	-0.001336	0.000527	0.001566
	DS* (-2 < x_f, y_f, z_f < 3)	-0.005274	0.008828	-0.006130	-0.001361	0.000522	0.001568
	DS* (-1 < x_f, y_f, z_f < 2)	-0.005328	0.008874	-0.006123	-0.001619	0.000517	0.001555
H12	Single molecule	-2.022337	-1.831442	-1.992187	0.018682	0.197380	-0.017769
	ES*	-0.007682	-0.017405	-0.008676	-0.002681	-0.005357	0.000184
	DS* (-4 < x_f, y_f, z_f < 5)	-0.007682	-0.017404	-0.008677	-0.002687	-0.005360	0.000187
	DS* (-3 < x_f, y_f, z_f < 4)	-0.007685	-0.017400	-0.008678	-0.002689	-0.005363	0.000189
	DS* (-2 < x_f, y_f, z_f < 3)	-0.007722	-0.017361	-0.008681	-0.002681	-0.005373	0.000195
	DS* (-1 < x_f, y_f, z_f < 2)	-0.007974	-0.016830	-0.008952	-0.002465	-0.005559	0.000330
H13	Single molecule	-1.972193	-1.889158	-2.733662	0.042900	-0.300228	0.133745
	ES*	0.000157	-0.001457	0.001111	-0.000269	0.000997	-0.000210
	DS* (-4 < x_f, y_f, z_f < 5)	0.000157	-0.001456	0.001109	-0.000274	0.000994	-0.000208
	DS* (-3 < x_f, y_f, z_f < 4)	0.000157	-0.001455	0.001108	-0.000279	0.000991	-0.000206
	DS* (-2 < x_f, y_f, z_f < 3)	0.000157	-0.001452	0.001106	-0.000299	0.000985	-0.000203
	DS* (-1 < x_f, y_f, z_f < 2)	0.000174	-0.001456	0.001093	-0.000495	0.000958	-0.000199

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H14	Single molecule	-2.666101	-1.902772	-1.902155	-0.063603	0.121400	0.014042
	ES*	0.001915	-0.004370	0.002278	-0.002133	-0.000822	0.001859
	DS* (-4 < x_f, y_f, z_f < 5)	0.001915	-0.004369	0.002276	-0.002139	-0.000826	0.001862
	DS* (-3 < x_f, y_f, z_f < 4)	0.001914	-0.004368	0.002275	-0.002143	-0.000828	0.001863
	DS* (-2 < x_f, y_f, z_f < 3)	0.001913	-0.004364	0.002273	-0.002165	-0.000834	0.001866
	DS* (-1 < x_f, y_f, z_f < 2)	0.001907	-0.004352	0.002267	-0.002378	-0.000864	0.001865
H15	Single molecule	-2.000285	-2.296199	-2.119198	0.170892	0.132849	-0.266265
	ES*	0.000045	0.000044	-0.000826	-0.000041	-0.002911	-0.000106
	DS* (-4 < x_f, y_f, z_f < 5)	0.000045	0.000045	-0.000828	-0.000046	-0.002914	-0.000103
	DS* (-3 < x_f, y_f, z_f < 4)	0.000045	0.000046	-0.000829	-0.000050	-0.002917	-0.000101
	DS* (-2 < x_f, y_f, z_f < 3)	0.000045	0.000048	-0.000831	-0.000070	-0.002922	-0.000099
	DS* (-1 < x_f, y_f, z_f < 2)	0.000061	0.000044	-0.000842	-0.000245	-0.002940	-0.000095

Table S9 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ACG** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-0.186659	0.127524	0.059135	-0.670968	1.366734	0.592703
	ES*	0.002671	-0.005764	0.003093	-0.001440	-0.006595	-0.000120
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002671	-0.005761	0.003090	-0.001448	-0.006600	-0.000116
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002668	-0.005757	0.003089	-0.001452	-0.006604	-0.000113
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002631	-0.005716	0.003086	-0.001446	-0.006617	-0.000105
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002124	-0.005168	0.003044	-0.001110	-0.006875	0.000013
O2	Single molecule	0.201048	-0.163359	-0.037689	0.863736	-1.254849	-0.774289
	ES*	0.004125	-0.005968	0.001843	0.007066	-0.000639	-0.006987
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004125	-0.005965	0.001841	0.007057	-0.000644	-0.006983
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004122	-0.005962	0.001839	0.007050	-0.000648	-0.006981
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004092	-0.005929	0.001837	0.007006	-0.000659	-0.006979
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003637	-0.005498	0.001861	0.006502	-0.000872	-0.007074
O3	Single molecule	0.027909	-0.069814	0.041906	0.936012	-0.881696	-0.919873
	ES*	-0.013696	0.020218	-0.006521	-0.001126	0.027681	0.002828
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.013697	0.020220	-0.006524	-0.001134	0.027676	0.002832
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.013697	0.020222	-0.006525	-0.001140	0.027673	0.002835
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.013696	0.020224	-0.006528	-0.001159	0.027664	0.002840
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.013678	0.020212	-0.006534	-0.001295	0.027633	0.002846
N4	Single molecule	0.093519	-0.303971	0.210452	0.093565	0.518341	-0.021163
	ES*	-0.002135	0.003684	-0.001549	0.000756	0.002618	0.000396
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002135	0.003686	-0.001551	0.000748	0.002613	0.000400
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002136	0.003688	-0.001553	0.000741	0.002609	0.000402
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002144	0.003701	-0.001556	0.000712	0.002600	0.000406
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002271	0.003828	-0.001557	0.000432	0.002579	0.000398
C5	Single molecule	-0.072645	0.214714	-0.142069	-0.108066	-0.478579	0.119242
	ES*	0.001732	-0.003009	0.001276	0.002044	-0.000416	-0.003073
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001732	-0.003006	0.001274	0.002036	-0.000421	-0.003069
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001729	-0.003002	0.001273	0.002030	-0.000424	-0.003066
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001697	-0.002966	0.001270	0.002010	-0.000436	-0.003062
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001123	-0.002442	0.001319	0.001876	-0.000626	-0.003066
C6	Single molecule	0.094407	-0.185340	0.090934	-0.080385	0.043455	0.095452
	ES*	0.000059	-0.000555	0.000496	0.001357	0.002630	-0.000636
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000058	-0.000552	0.000494	0.001349	0.002625	-0.000632
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000057	-0.000549	0.000493	0.001343	0.002621	-0.000629
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000040	-0.000529	0.000489	0.001326	0.002611	-0.000624
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000236	-0.000266	0.000502	0.001238	0.002567	-0.000619

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C7	Single molecule	-0.072531	0.249181	-0.176650	-0.138101	-0.364251	0.041932
	ES*	-0.001032	0.001009	0.000023	0.003067	0.005088	-0.001484
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001032	0.001012	0.000020	0.003059	0.005082	-0.001480
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001033	0.001014	0.000019	0.003052	0.005079	-0.001478
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001035	0.001020	0.000016	0.003025	0.005070	-0.001474
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001062	0.001056	0.000006	0.002779	0.005040	-0.001476
C8	Single molecule	-0.009012	0.055512	-0.046500	0.013266	0.000709	0.002258
	ES*	0.001111	-0.002681	0.001570	0.000056	-0.000022	0.000726
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001111	-0.002679	0.001568	0.000048	-0.000027	0.000730
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001110	-0.002677	0.001567	0.000041	-0.000031	0.000732
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001110	-0.002673	0.001563	0.000010	-0.000040	0.000736
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001117	-0.002666	0.001549	-0.000279	-0.000075	0.000738
H9	Single molecule	0.156089	0.016847	-0.172936	-0.143629	-0.185700	-0.286389
	ES*	0.000188	-0.000533	0.000345	0.000647	0.001758	0.002460
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000187	-0.000530	0.000343	0.000639	0.001752	0.002464
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000186	-0.000527	0.000341	0.000634	0.001749	0.002467
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000163	-0.000500	0.000337	0.000626	0.001738	0.002473
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000177	-0.000150	0.000327	0.000673	0.001714	0.002478
H10	Single molecule	-0.174327	0.056240	0.118087	0.267663	-0.234457	0.164024
	ES*	0.000345	-0.001763	0.001418	-0.000263	0.001428	-0.000105
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000345	-0.001760	0.001416	-0.000271	0.001423	-0.000101
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000344	-0.001758	0.001414	-0.000277	0.001420	-0.000099
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000337	-0.001747	0.001411	-0.000287	0.001411	-0.000092
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000227	-0.001633	0.001406	-0.000288	0.001367	-0.000069
H11	Single molecule	0.143421	-0.336469	0.193047	0.304195	0.179001	-0.256219
	ES*	-0.006616	0.014517	-0.007900	-0.001989	0.000800	0.002342
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.006617	0.014519	-0.007902	-0.001997	0.000795	0.002346
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.006617	0.014521	-0.007904	-0.002005	0.000791	0.002348
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.006622	0.014530	-0.007907	-0.002041	0.000783	0.002351
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006703	0.014600	-0.007897	-0.002428	0.000776	0.002333
H12	Single molecule	-0.110523	0.175820	-0.065297	0.028023	0.296070	-0.026654
	ES*	0.005359	-0.009226	0.003868	-0.004022	-0.008035	0.000276
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005358	-0.009224	0.003866	-0.004030	-0.008040	0.000280
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005354	-0.009219	0.003865	-0.004034	-0.008044	0.000283
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005298	-0.009159	0.003861	-0.004021	-0.008059	0.000292
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004917	-0.008367	0.003450	-0.003697	-0.008339	0.000495
H13	Single molecule	0.339217	0.463770	-0.802987	0.064349	-0.450342	0.200617
	ES*	0.000331	-0.002092	0.001761	-0.000403	0.001496	-0.000315
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000330	-0.002089	0.001759	-0.000411	0.001491	-0.000311
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000330	-0.002087	0.001757	-0.000418	0.001487	-0.000309
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000331	-0.002084	0.001753	-0.000449	0.001478	-0.000305
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000355	-0.002090	0.001734	-0.000743	0.001437	-0.000298

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H14	Single molecule	-0.763638	0.381356	0.382282	-0.095405	0.182101	0.021062
	ES*	0.002961	-0.006467	0.003505	-0.003200	-0.001233	0.002789
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002961	-0.006464	0.003503	-0.003208	-0.001239	0.002792
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002961	-0.006462	0.003502	-0.003215	-0.001242	0.002795
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002959	-0.006458	0.003499	-0.003248	-0.001251	0.002798
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002950	-0.006439	0.003489	-0.003566	-0.001296	0.002797
H15	Single molecule	0.207414	-0.236458	0.029045	0.256338	0.199273	-0.399398
	ES*	0.000436	0.000434	-0.000871	-0.000061	-0.004366	-0.000158
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000436	0.000437	-0.000873	-0.000069	-0.004371	-0.000155
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000436	0.000438	-0.000874	-0.000076	-0.004375	-0.000152
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000437	0.000441	-0.000878	-0.000105	-0.004383	-0.000148
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000460	0.000434	-0.000894	-0.000367	-0.004410	-0.000143

Table S10 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **ALA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.496442	0.246182	-0.167995	0.088532	0.310911
	ES*	0.096871	-0.001439	0.011625	-0.026413	0.028894
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.070716	-0.001437	0.011608	-0.026354	0.028833
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.070612	-0.001435	0.011597	-0.026314	0.028792
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.070338	-0.001433	0.011578	-0.026211	0.028690
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.068928	-0.001427	0.011644	-0.025703	0.028253
O2	Single molecule	-22.523593	-0.129442	0.107597	0.256937	0.307163
	ES*	0.139281	-0.001925	-0.009047	-0.030550	0.031920
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.113109	-0.001914	-0.009065	-0.030505	0.031881
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.112995	-0.001907	-0.009078	-0.030475	0.031856
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.112677	-0.001887	-0.009110	-0.030394	0.031786
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.110806	-0.001767	-0.009255	-0.029923	0.031371
N1	Single molecule	-18.313277	-0.026815	0.006624	0.041637	0.049966
	ES*	-0.040896	0.002949	-0.000064	-0.021408	0.021610
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.066798	0.002939	-0.000060	-0.021364	0.021566
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.066734	0.002933	-0.000057	-0.021336	0.021536
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.066593	0.002919	-0.000037	-0.021266	0.021466
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.066324	0.002894	0.000267	-0.020995	0.021195
C1	Single molecule	-14.797845	0.007648	-0.004515	0.051261	0.052025
	ES*	0.082603	-0.000323	-0.000612	-0.028449	0.028457
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.056489	-0.000319	-0.000626	-0.028400	0.028409
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.056412	-0.000316	-0.000634	-0.028367	0.028376
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.056198	-0.000307	-0.000652	-0.028283	0.028292
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.054931	-0.000254	-0.000654	-0.027861	0.027870
C2	Single molecule	-14.787464	-0.046913	0.027446	0.056041	0.078069
	ES*	0.012485	0.004216	0.001131	-0.023829	0.024226
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.013505	0.004215	0.001129	-0.023790	0.024187
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.013499	0.004214	0.001128	-0.023764	0.024161
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.013504	0.004215	0.001132	-0.023699	0.024098
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.013839	0.004246	0.001244	-0.023438	0.023852
C3	Single molecule	-14.842134	-0.026691	-0.014118	0.009097	0.031536
	ES*	0.012213	0.004935	-0.000339	-0.014805	0.015609
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.013752	0.004940	-0.000337	-0.014766	0.015574
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.013728	0.004942	-0.000335	-0.014740	0.015550
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.013676	0.004949	-0.000325	-0.014673	0.015489
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.013582	0.004969	-0.000190	-0.014363	0.015200

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H1	Single molecule	-0.933567	-0.002001	0.015317	0.023762	0.028341
	ES*	-0.052830	0.003040	-0.018264	-0.024649	0.030829
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.078729	0.003031	-0.018263	-0.024597	0.030785
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.078661	0.003026	-0.018261	-0.024561	0.030755
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.078487	0.003011	-0.018241	-0.024471	0.030669
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.077674	0.002946	-0.017932	-0.024032	0.030130
H2	Single molecule	-0.928181	-0.012376	-0.015567	0.011887	0.023169
	ES*	-0.050678	0.007003	0.017946	-0.014854	0.024326
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.076577	0.006990	0.017947	-0.014811	0.024297
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.076513	0.006981	0.017949	-0.014783	0.024279
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.076390	0.006964	0.017964	-0.014718	0.024245
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.076512	0.006958	0.018226	-0.014530	0.024325
H3	Single molecule	-0.904502	0.007879	-0.004953	0.023061	0.024868
	ES*	-0.082781	-0.006484	0.002104	-0.027705	0.028531
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.108620	-0.006497	0.002115	-0.027668	0.028499
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.108515	-0.006505	0.002124	-0.027644	0.028478
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.108283	-0.006524	0.002164	-0.027590	0.028433
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.107718	-0.006568	0.002648	-0.027392	0.028292
H4	Single molecule	-1.095668	-0.002050	-0.010646	0.025347	0.027568
	ES*	0.003229	0.003240	0.007201	-0.020796	0.022245
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.022753	0.003238	0.007201	-0.020766	0.022216
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.022743	0.003237	0.007201	-0.020746	0.022198
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.022744	0.003237	0.007204	-0.020701	0.022157
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.023186	0.003297	0.007253	-0.020590	0.022078
H5	Single molecule	-1.094130	-0.025042	-0.002618	-0.005176	0.025705
	ES*	-0.004413	0.012992	0.001807	-0.010737	0.016951
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.030314	0.012993	0.001817	-0.010705	0.016933
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.030249	0.012993	0.001824	-0.010684	0.016920
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.030095	0.012995	0.001853	-0.010632	0.016892
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.029604	0.012997	0.002114	-0.010418	0.016791
H6	Single molecule	-1.136561	-0.018543	-0.001165	0.024181	0.030495
	ES*	0.032531	-0.002778	-0.002333	-0.010263	0.010885
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.006525	-0.002767	-0.002335	-0.010226	0.010848
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.006521	-0.002760	-0.002336	-0.010202	0.010824
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.006500	-0.002743	-0.002337	-0.010139	0.010760
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.006218	-0.002671	-0.002333	-0.009836	0.010456
H7	Single molecule	-1.110507	-0.009143	-0.022340	0.013908	0.027859
	ES*	0.007797	0.003928	-0.002363	-0.015182	0.015859
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.018168	0.003933	-0.002362	-0.015135	0.015815
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.018144	0.003936	-0.002361	-0.015102	0.015784
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.018076	0.003942	-0.002350	-0.015016	0.015701
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.017709	0.003920	-0.002201	-0.014574	0.015252

Table S11 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ALA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.435477	-1306.320009	-1304.814028	0.112083	-0.170636	0.219935
	ES*	0.004178	-0.012984	0.006061	0.005412	0.001265	0.001230
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004176	-0.012984	0.006063	0.005411	0.001267	0.001226
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004175	-0.012984	0.006064	0.005410	0.001269	0.001223
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004171	-0.012984	0.006069	0.005410	0.001273	0.001216
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004156	-0.013010	0.006109	0.005432	0.001286	0.001188
O2	Single molecule	-1305.689640	-1306.054308	-1305.801681	-0.343424	0.726459	-0.472129
	ES*	0.000356	-0.003723	-0.001838	0.012683	-0.008307	0.002798
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000354	-0.003722	-0.001836	0.012682	-0.008304	0.002795
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000353	-0.003722	-0.001835	0.012681	-0.008303	0.002792
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000349	-0.003724	-0.001829	0.012681	-0.008299	0.002785
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000328	-0.003783	-0.001750	0.012693	-0.008279	0.002735
N1	Single molecule	-863.335013	-863.388448	-863.339860	-0.017042	-0.050561	0.011826
	ES*	-0.002548	0.004851	-0.002687	0.000917	0.002550	0.001210
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002550	0.004851	-0.002685	0.000916	0.002553	0.001206
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002552	0.004851	-0.002683	0.000916	0.002554	0.001203
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002555	0.004850	-0.002679	0.000915	0.002558	0.001193
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002560	0.004829	-0.002653	0.000933	0.002571	0.001102
C1	Single molecule	-534.031143	-534.228486	-533.956882	-0.286311	-0.045013	0.071513
	ES*	0.000802	-0.000068	-0.001083	0.002533	-0.000916	-0.001587
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000800	-0.000068	-0.001081	0.002532	-0.000913	-0.001591
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000799	-0.000067	-0.001080	0.002532	-0.000911	-0.001593
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000795	-0.000068	-0.001076	0.002531	-0.000907	-0.001601
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000780	-0.000106	-0.001024	0.002547	-0.000892	-0.001643
C2	Single molecule	-534.135745	-533.938633	-534.108564	0.064174	0.200069	-0.047309
	ES*	0.000453	0.001539	-0.002093	0.000402	-0.002014	-0.000137
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000451	0.001539	-0.002091	0.000401	-0.002012	-0.000141
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000450	0.001539	-0.002090	0.000401	-0.002010	-0.000144
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000446	0.001538	-0.002085	0.000400	-0.002006	-0.000153
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000433	0.001511	-0.002044	0.000416	-0.001989	-0.000218
C3	Single molecule	-533.510634	-533.512437	-533.517937	0.005985	0.004808	-0.000198
	ES*	0.000328	0.001174	-0.001606	0.000360	-0.003922	-0.000957
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000326	0.001174	-0.001604	0.000359	-0.003919	-0.000961
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000324	0.001175	-0.001603	0.000359	-0.003918	-0.000963
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000321	0.001174	-0.001599	0.000359	-0.003913	-0.000972
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000310	0.001163	-0.001577	0.000384	-0.003893	-0.001041

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H1	Single molecule	-1.828694	-2.207694	-1.773605	0.145065	-0.010790	0.042570
	ES*	-0.009775	0.012697	-0.010927	-0.003777	-0.000005	0.003390
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.009777	0.012697	-0.010925	-0.003778	-0.000003	0.003386
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.009778	0.012697	-0.010923	-0.003779	-0.000001	0.003383
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.009782	0.012698	-0.010920	-0.003779	0.000003	0.003373
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.009795	0.012711	-0.010920	-0.003758	0.000014	0.003294
H2	Single molecule	-2.059056	-1.966785	-1.783901	-0.231568	-0.052671	-0.046396
	ES*	-0.005003	0.009168	-0.012950	0.009832	0.003399	0.004334
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005005	0.009168	-0.012948	0.009831	0.003402	0.004330
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005006	0.009168	-0.012947	0.009830	0.003403	0.004328
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005009	0.009165	-0.012941	0.009830	0.003408	0.004318
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.005010	0.009115	-0.012890	0.009848	0.003417	0.004233
H3	Single molecule	-1.840726	-1.785472	-2.183533	0.022135	-0.160623	0.056798
	ES*	-0.005225	-0.007898	0.001206	-0.003872	0.010749	-0.003594
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005227	-0.007898	0.001208	-0.003873	0.010752	-0.003598
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005228	-0.007898	0.001209	-0.003874	0.010754	-0.003601
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005232	-0.007900	0.001215	-0.003874	0.010758	-0.003613
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.005224	-0.007919	0.001226	-0.003858	0.010772	-0.003745
H4	Single molecule	-1.970207	-2.328658	-1.949777	0.091947	0.001788	0.035921
	ES*	0.000290	0.005710	-0.007886	-0.002349	-0.001780	0.002040
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000288	0.005711	-0.007884	-0.002350	-0.001777	0.002037
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000287	0.005711	-0.007882	-0.002350	-0.001776	0.002034
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000283	0.005709	-0.007877	-0.002351	-0.001771	0.002026
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000264	0.005668	-0.007817	-0.002343	-0.001754	0.001964
H5	Single molecule	-2.057310	-2.000546	-2.409817	0.040632	-0.177607	0.108124
	ES*	-0.000465	0.000038	-0.000046	0.001275	-0.004289	-0.001362
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000467	0.000039	-0.000044	0.001274	-0.004287	-0.001366
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000469	0.000039	-0.000043	0.001274	-0.004285	-0.001369
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000472	0.000038	-0.000039	0.001274	-0.004281	-0.001379
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000489	0.000030	-0.000014	0.001305	-0.004255	-0.001482
H6	Single molecule	-2.256360	-1.988717	-2.221721	0.056804	0.265260	-0.057040
	ES*	0.002187	-0.000867	-0.001832	0.001134	-0.006991	-0.001331
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002185	-0.000867	-0.001830	0.001134	-0.006988	-0.001334
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002184	-0.000867	-0.001829	0.001133	-0.006986	-0.001337
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002180	-0.000867	-0.001825	0.001133	-0.006982	-0.001345
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002169	-0.000888	-0.001792	0.001171	-0.006966	-0.001395
H7	Single molecule	-2.011956	-2.484216	-1.971393	0.118478	0.001622	0.006918
	ES*	0.002387	0.001457	-0.004387	0.001499	-0.003471	-0.000522
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002385	0.001458	-0.004385	0.001498	-0.003468	-0.000526
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002383	0.001458	-0.004384	0.001498	-0.003467	-0.000529
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002381	0.001459	-0.004382	0.001497	-0.003462	-0.000538
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002378	0.001464	-0.004385	0.001512	-0.003443	-0.000595

Table S12 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **ALA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-0.868458	-0.695257	1.563715	0.168124	-0.255955	0.329902
	ES*	0.007640	-0.018104	0.010465	0.008117	0.001897	0.001845
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.007636	-0.018104	0.010467	0.008116	0.001901	0.001839
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.007634	-0.018103	0.010469	0.008115	0.001904	0.001835
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.007628	-0.018104	0.010475	0.008115	0.001910	0.001824
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.007606	-0.018142	0.010536	0.008147	0.001929	0.001782
O2	Single molecule	0.238355	-0.308648	0.070293	-0.515136	1.089689	-0.708194
	ES*	0.003137	-0.002982	-0.000155	0.019024	-0.012461	0.004198
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003134	-0.002982	-0.000152	0.019023	-0.012457	0.004192
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003131	-0.002981	-0.000150	0.019022	-0.012454	0.004188
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003126	-0.002984	-0.000142	0.019021	-0.012448	0.004177
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003094	-0.003072	-0.000022	0.019040	-0.012418	0.004103
N1	Single molecule	0.029141	-0.051011	0.021870	-0.025563	-0.075841	0.017739
	ES*	-0.003630	0.007468	-0.003838	0.001376	0.003825	0.001814
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003633	0.007468	-0.003835	0.001375	0.003829	0.001809
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003635	0.007468	-0.003833	0.001374	0.003831	0.001804
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003640	0.007466	-0.003826	0.001373	0.003837	0.001789
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003648	0.007435	-0.003787	0.001400	0.003856	0.001653
C1	Single molecule	0.061542	-0.234474	0.172932	-0.429466	-0.067520	0.107270
	ES*	0.001378	0.000073	-0.001450	0.003800	-0.001373	-0.002380
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001375	0.000073	-0.001448	0.003798	-0.001369	-0.002386
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001372	0.000073	-0.001446	0.003798	-0.001367	-0.002390
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001367	0.000072	-0.001439	0.003797	-0.001361	-0.002401
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001345	0.000016	-0.001361	0.003820	-0.001338	-0.002465
C2	Single molecule	-0.112147	0.183521	-0.071375	0.096262	0.300104	-0.070963
	ES*	0.000730	0.002359	-0.003089	0.000604	-0.003021	-0.000206
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000727	0.002359	-0.003086	0.000602	-0.003018	-0.000212
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000725	0.002359	-0.003084	0.000601	-0.003015	-0.000216
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000720	0.002358	-0.003077	0.000601	-0.003009	-0.000229
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000699	0.002317	-0.003016	0.000624	-0.002983	-0.000328
C3	Single molecule	0.004553	0.001849	-0.006402	0.008978	0.007213	-0.000296
	ES*	0.000544	0.001813	-0.002357	0.000541	-0.005883	-0.001435
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000541	0.001814	-0.002354	0.000539	-0.005879	-0.001441
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000539	0.001814	-0.002352	0.000538	-0.005876	-0.001445
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000534	0.001813	-0.002347	0.000538	-0.005870	-0.001459
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000517	0.001796	-0.002313	0.000576	-0.005840	-0.001561

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H1	Single molecule	0.161956	-0.406544	0.244589	0.217597	-0.016185	0.063856
	ES*	-0.010660	0.023047	-0.012387	-0.005666	-0.000008	0.005084
	DS* (-4 < x_f, y_f, z_f < 5)	-0.010663	0.023048	-0.012385	-0.005667	-0.000004	0.005079
	DS* (-3 < x_f, y_f, z_f < 4)	-0.010665	0.023048	-0.012383	-0.005668	-0.000002	0.005074
	DS* (-2 < x_f, y_f, z_f < 3)	-0.010671	0.023049	-0.012378	-0.005668	0.000004	0.005059
	DS* (-1 < x_f, y_f, z_f < 2)	-0.010690	0.023069	-0.012378	-0.005637	0.000021	0.004941
H2	Single molecule	-0.183713	-0.045307	0.229020	-0.347352	-0.079006	-0.069594
	ES*	-0.003111	0.018144	-0.015033	0.014748	0.005099	0.006501
	DS* (-4 < x_f, y_f, z_f < 5)	-0.003115	0.018145	-0.015030	0.014746	0.005103	0.006495
	DS* (-3 < x_f, y_f, z_f < 4)	-0.003117	0.018145	-0.015028	0.014746	0.005105	0.006491
	DS* (-2 < x_f, y_f, z_f < 3)	-0.003121	0.018141	-0.015019	0.014745	0.005111	0.006477
	DS* (-1 < x_f, y_f, z_f < 2)	-0.003123	0.018065	-0.014942	0.014772	0.005125	0.006349
H3	Single molecule	0.143777	0.226658	-0.370435	0.033202	-0.240934	0.085198
	ES*	-0.001879	-0.005888	0.007767	-0.005808	0.016124	-0.005391
	DS* (-4 < x_f, y_f, z_f < 5)	-0.001882	-0.005888	0.007770	-0.005809	0.016128	-0.005397
	DS* (-3 < x_f, y_f, z_f < 4)	-0.001884	-0.005888	0.007772	-0.005810	0.016131	-0.005401
	DS* (-2 < x_f, y_f, z_f < 3)	-0.001889	-0.005892	0.007781	-0.005811	0.016137	-0.005419
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001878	-0.005920	0.007798	-0.005787	0.016158	-0.005617
H4	Single molecule	0.169010	-0.368666	0.199656	0.137921	0.002682	0.053882
	ES*	0.001378	0.009508	-0.010886	-0.003523	-0.002670	0.003061
	DS* (-4 < x_f, y_f, z_f < 5)	0.001375	0.009508	-0.010883	-0.003525	-0.002666	0.003055
	DS* (-3 < x_f, y_f, z_f < 4)	0.001373	0.009509	-0.010881	-0.003526	-0.002663	0.003051
	DS* (-2 < x_f, y_f, z_f < 3)	0.001367	0.009506	-0.010873	-0.003527	-0.002657	0.003039
	DS* (-1 < x_f, y_f, z_f < 2)	0.001338	0.009445	-0.010783	-0.003514	-0.002630	0.002946
H5	Single molecule	0.147871	0.233018	-0.380889	0.060948	-0.266410	0.162187
	ES*	-0.000461	0.000294	0.000167	0.001913	-0.006434	-0.002043
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000464	0.000294	0.000170	0.001911	-0.006430	-0.002049
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000466	0.000294	0.000172	0.001911	-0.006428	-0.002053
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000471	0.000293	0.000178	0.001911	-0.006421	-0.002069
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000497	0.000282	0.000215	0.001958	-0.006383	-0.002223
H6	Single molecule	-0.151141	0.250323	-0.099182	0.085206	0.397890	-0.085560
	ES*	0.003537	-0.001045	-0.002492	0.001702	-0.010486	-0.001996
	DS* (-4 < x_f, y_f, z_f < 5)	0.003534	-0.001045	-0.002489	0.001700	-0.010482	-0.002002
	DS* (-3 < x_f, y_f, z_f < 4)	0.003531	-0.001044	-0.002487	0.001699	-0.010479	-0.002006
	DS* (-2 < x_f, y_f, z_f < 3)	0.003526	-0.001045	-0.002481	0.001700	-0.010473	-0.002018
	DS* (-1 < x_f, y_f, z_f < 2)	0.003509	-0.001077	-0.002432	0.001756	-0.010449	-0.002093
H7	Single molecule	0.215849	-0.492541	0.276693	0.177716	0.002433	0.010376
	ES*	0.003852	0.002457	-0.006309	0.002249	-0.005207	-0.000783
	DS* (-4 < x_f, y_f, z_f < 5)	0.003848	0.002458	-0.006306	0.002248	-0.005203	-0.000789
	DS* (-3 < x_f, y_f, z_f < 4)	0.003846	0.002458	-0.006305	0.002247	-0.005200	-0.000793
	DS* (-2 < x_f, y_f, z_f < 3)	0.003842	0.002459	-0.006301	0.002246	-0.005194	-0.000807
	DS* (-1 < x_f, y_f, z_f < 2)	0.003839	0.002467	-0.006306	0.002268	-0.005164	-0.000892

Table S13 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **BENZ** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the atoms of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C1	Single molecule	-14.86385	0.00723	0.02260	-0.00037	0.02373
	ES*	0.05357	-0.00049	-0.00149	0.00019	0.00158
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07006	-0.00046	-0.00147	0.00018	0.00155
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07007	-0.00045	-0.00146	0.00018	0.00153
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07009	-0.00040	-0.00142	0.00017	0.00149
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07021	-0.00025	-0.00131	0.00015	0.00135
C2	Single molecule	-14.86355	0.01631	0.00716	0.01630	0.02414
	ES*	0.05018	-0.00316	0.00080	-0.00279	0.00429
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06664	-0.00313	0.00082	-0.00280	0.00428
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06664	-0.00311	0.00083	-0.00280	0.00427
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06664	-0.00306	0.00087	-0.00282	0.00425
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06671	-0.00292	0.00098	-0.00283	0.00418
C3	Single molecule	-14.86411	-0.00996	0.01398	-0.01408	0.02220
	ES*	0.05102	0.00196	-0.00046	0.00271	0.00337
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06745	0.00198	-0.00044	0.00270	0.00338
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06743	0.00199	-0.00044	0.00269	0.00338
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06738	0.00203	-0.00041	0.00267	0.00338
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06723	0.00215	-0.00034	0.00262	0.00340
H1	Single molecule	-1.12743	-0.00368	0.00152	-0.00884	0.00969
	ES*	0.04751	-0.00122	-0.00431	0.00050	0.00451
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06406	-0.00119	-0.00429	0.00050	0.00448
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06412	-0.00117	-0.00427	0.00050	0.00445
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06425	-0.00112	-0.00423	0.00051	0.00440
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06471	-0.00096	-0.00408	0.00050	0.00422
H2	Single molecule	-1.12754	0.00393	-0.00334	-0.00146	0.00536
	ES*	0.03987	-0.00550	0.00341	-0.00513	0.00825
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05639	-0.00546	0.00344	-0.00513	0.00825
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05643	-0.00544	0.00346	-0.00513	0.00824
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05652	-0.00538	0.00350	-0.00514	0.00822
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05684	-0.00526	0.00363	-0.00517	0.00823
H3	Single molecule	-1.12800	-0.00080	-0.00020	-0.00252	0.00265
	ES*	0.04476	0.00161	0.00070	0.00389	0.00426
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06121	0.00163	0.00072	0.00388	0.00427
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06119	0.00164	0.00072	0.00387	0.00427
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06117	0.00167	0.00075	0.00386	0.00427
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06108	0.00177	0.00082	0.00381	0.00428

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
X5_C1	Single molecule	-14.86385	-0.00723	-0.02260	0.00037	0.02373
	ES*	0.05357	0.00049	0.00149	-0.00019	0.00158
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06994	0.00051	0.00150	-0.00021	0.00160
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06988	0.00053	0.00151	-0.00023	0.00161
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06972	0.00056	0.00152	-0.00026	0.00164
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06920	0.00069	0.00158	-0.00038	0.00176
X5_C2	Single molecule	-14.86355	-0.01631	-0.00716	-0.01630	0.02414
	ES*	0.05018	0.00316	-0.00080	0.00279	0.00429
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06657	0.00318	-0.00079	0.00277	0.00429
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06652	0.00319	-0.00079	0.00275	0.00429
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06641	0.00322	-0.00078	0.00272	0.00429
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06602	0.00333	-0.00074	0.00262	0.00430
X5_C3	Single molecule	-14.86411	0.00996	-0.01398	0.01408	0.02220
	ES*	0.05102	-0.00196	0.00046	-0.00271	0.00337
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06741	-0.00193	0.00047	-0.00273	0.00337
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06736	-0.00191	0.00048	-0.00274	0.00337
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06725	-0.00186	0.00051	-0.00277	0.00337
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06693	-0.00172	0.00062	-0.00281	0.00336
X5_H1	Single molecule	-1.12743	0.00368	-0.00152	0.00884	0.00969
	ES*	0.04751	0.00122	0.00431	-0.00050	0.00451
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06385	0.00124	0.00432	-0.00053	0.00452
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06377	0.00125	0.00432	-0.00055	0.00453
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06358	0.00129	0.00432	-0.00060	0.00455
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06286	0.00140	0.00435	-0.00078	0.00464
X5_H2	Single molecule	-1.12754	-0.00393	0.00334	0.00146	0.00536
	ES*	0.03987	0.00550	-0.00341	0.00513	0.00825
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05626	0.00551	-0.00341	0.00510	0.00825
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05622	0.00552	-0.00341	0.00509	0.00824
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05611	0.00554	-0.00341	0.00505	0.00824
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05571	0.00562	-0.00341	0.00491	0.00821
X5_H3	Single molecule	-1.12800	0.00080	0.00020	0.00252	0.00265
	ES*	0.04476	-0.00161	-0.00070	-0.00389	0.00426
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06113	-0.00158	-0.00069	-0.00391	0.00427
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06107	-0.00155	-0.00068	-0.00392	0.00427
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06092	-0.00150	-0.00065	-0.00395	0.00428
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06046	-0.00136	-0.00048	-0.00403	0.00428

Table S14 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **BENZ** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C1	Single molecule	-534.296720	-534.173834	-534.271621	0.050628	0.200043	-0.065719
	ES*	-0.000399	0.000851	-0.000550	0.000493	0.001707	-0.000843
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000398	0.000848	-0.000548	0.000492	0.001703	-0.000845
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000398	0.000847	-0.000546	0.000491	0.001701	-0.000846
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000397	0.000842	-0.000543	0.000489	0.001695	-0.000849
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000389	0.000829	-0.000538	0.000481	0.001677	-0.000853
C2	Single molecule	-534.326912	-534.112563	-534.304097	0.050354	0.167623	-0.079587
	ES*	0.000187	-0.000298	0.000017	-0.000029	0.001790	-0.001035
	DS* (-4 < x_f, y_f, z_f < 5)	0.000188	-0.000300	0.000020	-0.000030	0.001786	-0.001038
	DS* (-3 < x_f, y_f, z_f < 4)	0.000188	-0.000302	0.000021	-0.000031	0.001783	-0.001039
	DS* (-2 < x_f, y_f, z_f < 3)	0.000188	-0.000306	0.000024	-0.000033	0.001777	-0.001042
	DS* (-1 < x_f, y_f, z_f < 2)	0.000202	-0.000307	0.000013	-0.000041	0.001780	-0.001045
C3	Single molecule	-534.296286	-534.138911	-534.311229	0.090085	0.178411	-0.039200
	ES*	-0.000249	0.000054	0.000103	0.001014	0.001649	-0.000199
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000248	0.000051	0.000106	0.001013	0.001645	-0.000202
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000248	0.000049	0.000107	0.001012	0.001643	-0.000203
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000247	0.000045	0.000111	0.001010	0.001637	-0.000207
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000241	0.000032	0.000118	0.001003	0.001613	-0.000216
H1	Single molecule	-1.978387	-2.368134	-1.940649	-0.132588	-0.000718	0.031972
	ES*	-0.000340	0.001249	-0.001246	0.000730	0.001583	-0.000377
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000340	0.001247	-0.001244	0.000728	0.001579	-0.000379
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000340	0.001245	-0.001242	0.000727	0.001577	-0.000381
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000339	0.001241	-0.001238	0.000726	0.001571	-0.000384
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000335	0.001222	-0.001223	0.000716	0.001552	-0.000389
H2	Single molecule	-2.186101	-1.989475	-2.112831	-0.104928	-0.216813	-0.081454
	ES*	-0.000004	-0.001334	0.000492	-0.000661	0.001835	-0.001344
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000004	-0.001336	0.000495	-0.000662	0.001831	-0.001346
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000004	-0.001338	0.000496	-0.000663	0.001829	-0.001348
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000004	-0.001342	0.000500	-0.000665	0.001823	-0.001351
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000007	-0.001352	0.000513	-0.000680	0.001855	-0.001348
H3	Single molecule	-2.018970	-2.132973	-2.137698	0.117168	-0.135006	0.194192
	ES*	-0.000383	0.000595	-0.000673	0.002760	0.001448	0.000077
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000383	0.000593	-0.000671	0.002758	0.001444	0.000074
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000382	0.000591	-0.000669	0.002757	0.001442	0.000073
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000382	0.000587	-0.000666	0.002755	0.001436	0.000069
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000378	0.000571	-0.000654	0.002749	0.001413	0.000058

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
X5_C1	Single molecule	-534.296720	-534.173834	-534.271621	0.050628	0.200043	-0.065719
	ES*	-0.000399	0.000851	-0.000550	0.000493	0.001707	-0.000843
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000398	0.000848	-0.000548	0.000492	0.001703	-0.000845
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000398	0.000847	-0.000546	0.000491	0.001701	-0.000846
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000397	0.000843	-0.000543	0.000489	0.001695	-0.000850
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000390	0.000834	-0.000541	0.000479	0.001672	-0.000873
X5_C2	Single molecule	-534.326912	-534.112563	-534.304097	0.050354	0.167623	-0.079587
	ES*	0.000187	-0.000298	0.000017	-0.000029	0.001790	-0.001035
	DS* (-4 < x_f, y_f, z_f < 5)	0.000188	-0.000300	0.000020	-0.000030	0.001786	-0.001038
	DS* (-3 < x_f, y_f, z_f < 4)	0.000188	-0.000302	0.000021	-0.000031	0.001783	-0.001039
	DS* (-2 < x_f, y_f, z_f < 3)	0.000189	-0.000306	0.000024	-0.000033	0.001777	-0.001043
	DS* (-1 < x_f, y_f, z_f < 2)	0.000194	-0.000318	0.000031	-0.000041	0.001752	-0.001056
X5_C3	Single molecule	-534.296286	-534.138911	-534.311229	0.090085	0.178411	-0.039200
	ES*	-0.000249	0.000054	0.000103	0.001014	0.001649	-0.000199
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000248	0.000051	0.000106	0.001013	0.001645	-0.000202
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000248	0.000050	0.000107	0.001012	0.001643	-0.000203
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000248	0.000046	0.000110	0.001010	0.001637	-0.000207
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000234	0.000050	0.000093	0.001010	0.001630	-0.000236
X5_H1	Single molecule	-1.978387	-2.368134	-1.940649	-0.132588	-0.000718	0.031972
	ES*	-0.000340	0.001249	-0.001246	0.000730	0.001583	-0.000377
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000340	0.001247	-0.001244	0.000728	0.001579	-0.000379
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000340	0.001245	-0.001242	0.000727	0.001577	-0.000381
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000339	0.001241	-0.001239	0.000725	0.001570	-0.000384
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000337	0.001225	-0.001225	0.000712	0.001551	-0.000409
X5_H2	Single molecule	-2.186101	-1.989475	-2.112831	-0.104928	-0.216813	-0.081454
	ES*	-0.000004	-0.001334	0.000492	-0.000661	0.001835	-0.001344
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000004	-0.001336	0.000494	-0.000662	0.001831	-0.001346
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000004	-0.001338	0.000496	-0.000663	0.001829	-0.001348
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000003	-0.001342	0.000499	-0.000665	0.001823	-0.001352
	DS* (-1 < x_f, y_f, z_f < 2)	0.000001	-0.001357	0.000510	-0.000673	0.001798	-0.001364
X5_H3	Single molecule	-2.018970	-2.132973	-2.137698	0.117168	-0.135006	0.194192
	ES*	-0.000383	0.000595	-0.000673	0.002760	0.001448	0.000077
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000383	0.000593	-0.000671	0.002758	0.001444	0.000074
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000382	0.000591	-0.000669	0.002757	0.001442	0.000073
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000382	0.000588	-0.000666	0.002755	0.001436	0.000070
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000378	0.000586	-0.000669	0.002780	0.001437	0.000014

Table S15 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **BENZ** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C1	Single molecule	-0.073992	0.110336	-0.036344	0.075943	0.300065	-0.098578
	ES*	-0.000549	0.001325	-0.000776	0.000740	0.002560	-0.001264
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000548	0.001321	-0.000773	0.000738	0.002555	-0.001267
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000548	0.001319	-0.000771	0.000736	0.002551	-0.001269
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000547	0.001312	-0.000765	0.000733	0.002542	-0.001274
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000535	0.001292	-0.000758	0.000721	0.002516	-0.001280
C2	Single molecule	-0.118582	0.202941	-0.084360	0.075531	0.251435	-0.119380
	ES*	0.000327	-0.000400	0.000073	-0.000043	0.002684	-0.001553
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000328	-0.000404	0.000076	-0.000045	0.002679	-0.001556
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000328	-0.000406	0.000078	-0.000046	0.002675	-0.001558
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000329	-0.000412	0.000083	-0.000049	0.002666	-0.001563
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000349	-0.000414	0.000065	-0.000062	0.002670	-0.001568
C3	Single molecule	-0.071216	0.164847	-0.093631	0.135127	0.267617	-0.058800
	ES*	-0.000327	0.000126	0.000201	0.001521	0.002473	-0.000299
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000327	0.000122	0.000204	0.001519	0.002468	-0.000303
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000326	0.000120	0.000206	0.001518	0.002464	-0.000305
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000325	0.000114	0.000212	0.001515	0.002455	-0.000310
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000316	0.000093	0.000223	0.001505	0.002420	-0.000324
H1	Single molecule	0.176004	-0.408616	0.232612	-0.198881	-0.001078	0.047957
	ES*	-0.000342	0.002042	-0.001700	0.001094	0.002374	-0.000565
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000342	0.002038	-0.001697	0.001092	0.002369	-0.000569
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000341	0.002036	-0.001695	0.001091	0.002365	-0.000571
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000340	0.002029	-0.001689	0.001088	0.002356	-0.000576
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000334	0.002001	-0.001667	0.001074	0.002327	-0.000583
H2	Single molecule	-0.134947	0.159991	-0.025043	-0.157392	-0.325219	-0.122181
	ES*	0.000416	-0.001578	0.001161	-0.000992	0.002753	-0.002016
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000417	-0.001582	0.001165	-0.000994	0.002747	-0.002020
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000417	-0.001584	0.001167	-0.000995	0.002743	-0.002022
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000418	-0.001590	0.001172	-0.000998	0.002734	-0.002026
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000412	-0.001605	0.001193	-0.001021	0.002783	-0.002021
H3	Single molecule	0.116365	-0.054639	-0.061726	0.175752	-0.202509	0.291288
	ES*	-0.000344	0.001123	-0.000779	0.004140	0.002172	0.000115
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000344	0.001119	-0.000776	0.004138	0.002166	0.000112
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000343	0.001117	-0.000774	0.004136	0.002163	0.000109
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000342	0.001110	-0.000768	0.004133	0.002154	0.000104
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000337	0.001087	-0.000750	0.004123	0.002119	0.000087

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
X5_C1	Single molecule	-0.073992	0.110336	-0.036344	0.075943	0.300065	-0.098578
	ES*	-0.000549	0.001325	-0.000776	0.000740	0.002560	-0.001264
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000548	0.001321	-0.000773	0.000738	0.002555	-0.001267
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000548	0.001319	-0.000771	0.000736	0.002551	-0.001269
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000547	0.001313	-0.000766	0.000733	0.002542	-0.001275
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000536	0.001300	-0.000764	0.000719	0.002508	-0.001309
X5_C2	Single molecule	-0.118582	0.202941	-0.084360	0.075531	0.251435	-0.119380
	ES*	0.000327	-0.000400	0.000073	-0.000043	0.002684	-0.001553
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000328	-0.000404	0.000076	-0.000045	0.002678	-0.001556
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000329	-0.000406	0.000078	-0.000046	0.002675	-0.001559
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000330	-0.000413	0.000083	-0.000049	0.002666	-0.001564
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000338	-0.000431	0.000093	-0.000062	0.002629	-0.001584
X5_C3	Single molecule	-0.071216	0.164847	-0.093631	0.135127	0.267617	-0.058800
	ES*	-0.000327	0.000126	0.000201	0.001521	0.002473	-0.000299
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000327	0.000123	0.000204	0.001519	0.002468	-0.000303
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000326	0.000120	0.000206	0.001518	0.002464	-0.000305
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000326	0.000114	0.000211	0.001515	0.002455	-0.000310
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000305	0.000120	0.000185	0.001515	0.002445	-0.000354
X5_H1	Single molecule	0.176004	-0.408616	0.232612	-0.198881	-0.001078	0.047957
	ES*	-0.000342	0.002042	-0.001700	0.001094	0.002374	-0.000565
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000342	0.002039	-0.001697	0.001092	0.002369	-0.000569
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000341	0.002036	-0.001695	0.001091	0.002365	-0.000571
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000340	0.002030	-0.001690	0.001088	0.002356	-0.000577
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000337	0.002006	-0.001669	0.001068	0.002326	-0.000613
X5_H2	Single molecule	-0.134947	0.159991	-0.025043	-0.157392	-0.325219	-0.122181
	ES*	0.000416	-0.001578	0.001161	-0.000992	0.002753	-0.002016
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000417	-0.001582	0.001165	-0.000994	0.002747	-0.002020
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000417	-0.001584	0.001167	-0.000995	0.002743	-0.002022
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000418	-0.001590	0.001172	-0.000998	0.002734	-0.002027
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000424	-0.001612	0.001189	-0.001010	0.002698	-0.002046
X5_H3	Single molecule	0.116365	-0.054639	-0.061726	0.175752	-0.202509	0.291288
	ES*	-0.000344	0.001123	-0.000779	0.004140	0.002172	0.000115
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000344	0.001120	-0.000776	0.004138	0.002166	0.000112
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000343	0.001117	-0.000774	0.004136	0.002163	0.000109
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000343	0.001112	-0.000769	0.004133	0.002154	0.000104
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000337	0.001110	-0.000773	0.004169	0.002156	0.000021

Table S16 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **GLY** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.49335	0.16099	-0.08615	0.24730	0.30741
	ES*	0.10786	0.01859	0.00462	-0.03289	0.03806
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06963	0.01880	0.00466	-0.03293	0.03820
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07013	0.01894	0.00469	-0.03296	0.03830
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07162	0.01928	0.00479	-0.03306	0.03857
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.08084	0.02069	0.00519	-0.03422	0.04032
O2	Single molecule	-22.51980	-0.29369	0.03782	0.09269	0.31029
	ES*	0.13282	0.01897	0.01262	-0.00883	0.02443
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.09530	0.01920	0.01267	-0.00894	0.02468
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.09627	0.01935	0.01271	-0.00900	0.02484
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.09895	0.01978	0.01288	-0.00915	0.02531
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.11388	0.02250	0.01399	-0.00968	0.02821
N1	Single molecule	-18.31023	-0.05060	0.02557	0.01847	0.05963
	ES*	-0.04028	0.01659	0.00003	-0.01558	0.02276
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.07905	0.01671	0.00003	-0.01564	0.02289
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.07891	0.01679	0.00004	-0.01568	0.02297
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.07839	0.01700	0.00007	-0.01578	0.02320
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.07459	0.01797	0.00038	-0.01620	0.02420
C1	Single molecule	-14.79395	-0.02401	-0.00366	0.04526	0.05137
	ES*	0.08456	0.01765	0.00322	-0.02416	0.03010
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04652	0.01785	0.00326	-0.02424	0.03028
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04715	0.01799	0.00329	-0.02429	0.03040
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04893	0.01834	0.00340	-0.02441	0.03072
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05875	0.02017	0.00418	-0.02515	0.03251
C2	Single molecule	-14.80495	-0.05855	0.02346	0.02741	0.06877
	ES*	0.00900	0.01817	0.00206	-0.01758	0.02537
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.02944	0.01831	0.00208	-0.01767	0.02553
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.02907	0.01841	0.00210	-0.01772	0.02564
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.02798	0.01870	0.00219	-0.01785	0.02594
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.02170	0.02013	0.00295	-0.01832	0.02738
H1	Single molecule	-0.90108	-0.01025	0.00592	0.02597	0.02854
	ES*	-0.08343	0.01883	0.00104	-0.02384	0.03039
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.12239	0.01891	0.00103	-0.02391	0.03050
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.12236	0.01896	0.00103	-0.02395	0.03057
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.12215	0.01912	0.00105	-0.02406	0.03075
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.11961	0.01995	0.00131	-0.02437	0.03153

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H2	Single molecule	-0.92446	-0.02019	0.00464	0.01740	0.02706
	ES*	-0.05105	0.02246	0.00619	-0.00653	0.02419
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.08993	0.02257	0.00620	-0.00655	0.02431
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.08986	0.02265	0.00621	-0.00657	0.02438
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.08957	0.02284	0.00626	-0.00662	0.02459
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.08672	0.02363	0.00677	-0.00703	0.02557
H3	Single molecule	-0.92011	-0.01082	0.00861	0.00939	0.01671
	ES*	-0.04240	0.01257	-0.01257	-0.01385	0.02254
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.08112	0.01271	-0.01257	-0.01392	0.02265
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.08093	0.01280	-0.01257	-0.01396	0.02273
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.08031	0.01303	-0.01256	-0.01408	0.02293
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.07601	0.01400	-0.01268	-0.01462	0.02389
H4	Single molecule	-1.08550	-0.01454	0.00861	0.00617	0.01799
	ES*	-0.01094	0.01791	0.00856	-0.01556	0.02522
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.04949	0.01804	0.00858	-0.01563	0.02537
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.04920	0.01813	0.00860	-0.01568	0.02547
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.04841	0.01837	0.00872	-0.01579	0.02574
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.04463	0.01943	0.00993	-0.01616	0.02716
H5	Single molecule	-1.08939	-0.01191	0.00449	0.01537	0.01995
	ES*	0.01229	0.01678	0.00069	-0.01440	0.02212
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.02608	0.01692	0.00071	-0.01452	0.02231
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.02566	0.01703	0.00073	-0.01460	0.02244
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.02429	0.01735	0.00081	-0.01475	0.02279
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.01597	0.01917	0.00132	-0.01516	0.02448

Table S17 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **GLY** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1305.49559	-1306.23992	-1305.69916	0.05251	-0.86502	0.05614
	ES*	-0.00136	0.00503	-0.00731	0.00277	0.00721	0.00004
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00137	0.00503	-0.00730	0.00277	0.00722	0.00004
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00138	0.00504	-0.00730	0.00277	0.00723	0.00005
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00140	0.00506	-0.00730	0.00276	0.00725	0.00006
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00163	0.00566	-0.00766	0.00280	0.00724	-0.00005
O2	Single molecule	-1306.43850	-1306.12789	-1304.86515	-0.02177	0.28289	-0.36873
	ES*	-0.00034	-0.00148	-0.00189	-0.00543	-0.01264	0.00193
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00035	-0.00147	-0.00188	-0.00543	-0.01263	0.00194
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00036	-0.00147	-0.00187	-0.00544	-0.01262	0.00194
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00039	-0.00143	-0.00187	-0.00545	-0.01261	0.00195
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00092	-0.00070	-0.00207	-0.00551	-0.01289	0.00202
N1	Single molecule	-863.25739	-863.32009	-863.33447	-0.04580	-0.02190	0.00874
	ES*	-0.00159	0.00283	-0.00174	0.00026	0.00041	-0.00037
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00160	0.00284	-0.00172	0.00026	0.00043	-0.00036
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00161	0.00284	-0.00172	0.00026	0.00044	-0.00036
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00164	0.00286	-0.00171	0.00025	0.00045	-0.00035
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00181	0.00309	-0.00177	0.00025	0.00048	-0.00029
C1	Single molecule	-533.81586	-534.36967	-533.98407	-0.12060	0.03623	-0.11193
	ES*	-0.00167	0.00329	-0.00217	-0.00114	-0.00213	0.00276
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00168	0.00330	-0.00216	-0.00115	-0.00211	0.00276
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00169	0.00330	-0.00216	-0.00115	-0.00210	0.00277
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00171	0.00332	-0.00215	-0.00116	-0.00209	0.00278
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00203	0.00379	-0.00231	-0.00119	-0.00210	0.00282
C2	Single molecule	-534.01862	-533.81849	-533.72457	0.14097	0.04937	-0.03717
	ES*	-0.00033	0.00335	-0.00319	0.00026	-0.00006	-0.00022
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00034	0.00335	-0.00318	0.00026	-0.00004	-0.00022
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00035	0.00336	-0.00317	0.00026	-0.00003	-0.00021
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00038	0.00338	-0.00316	0.00024	-0.00002	-0.00020
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00064	0.00371	-0.00323	0.00016	0.00003	-0.00016
H1	Single molecule	-1.80982	-1.77974	-2.18741	-0.02145	0.13060	0.06738
	ES*	-0.00883	-0.00890	0.00474	-0.00320	-0.00774	-0.00016
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00884	-0.00890	0.00475	-0.00320	-0.00772	-0.00016
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00885	-0.00890	0.00476	-0.00321	-0.00772	-0.00016
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00888	-0.00888	0.00477	-0.00321	-0.00770	-0.00015
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00906	-0.00866	0.00474	-0.00323	-0.00769	-0.00011

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H2	Single molecule	-2.01656	-1.82755	-1.96444	-0.12334	-0.23320	-0.11323
	ES*	-0.00247	-0.00486	-0.00189	0.00227	0.01302	0.00710
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00248	-0.00486	-0.00188	0.00227	0.01304	0.00711
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00249	-0.00486	-0.00187	0.00226	0.01305	0.00711
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00252	-0.00484	-0.00186	0.00226	0.01307	0.00713
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00266	-0.00462	-0.00193	0.00226	0.01311	0.00721
H3	Single molecule	-1.77066	-2.26266	-1.77265	-0.05183	0.00643	0.08034
	ES*	0.00242	0.00891	-0.01583	0.00453	-0.00482	-0.00386
	DS* (-4 < x_f, y_f, z_f < 5)	0.00240	0.00891	-0.01582	0.00453	-0.00481	-0.00385
	DS* (-3 < x_f, y_f, z_f < 4)	0.00239	0.00891	-0.01581	0.00453	-0.00480	-0.00385
	DS* (-2 < x_f, y_f, z_f < 3)	0.00237	0.00893	-0.01580	0.00452	-0.00478	-0.00384
	DS* (-1 < x_f, y_f, z_f < 2)	0.00220	0.00914	-0.01585	0.00455	-0.00475	-0.00379
H4	Single molecule	-1.94214	-2.36833	-1.92053	-0.05612	0.01428	0.06237
	ES*	0.00360	0.00337	-0.00869	-0.00111	-0.00263	0.00105
	DS* (-4 < x_f, y_f, z_f < 5)	0.00359	0.00337	-0.00868	-0.00112	-0.00262	0.00105
	DS* (-3 < x_f, y_f, z_f < 4)	0.00358	0.00337	-0.00867	-0.00112	-0.00261	0.00105
	DS* (-2 < x_f, y_f, z_f < 3)	0.00355	0.00338	-0.00865	-0.00114	-0.00259	0.00106
	DS* (-1 < x_f, y_f, z_f < 2)	0.00342	0.00354	-0.00867	-0.00135	-0.00250	0.00108
H5	Single molecule	-2.11743	-1.97352	-2.11869	-0.08844	-0.18876	-0.10653
	ES*	-0.00012	0.00140	-0.00188	0.00236	0.00270	-0.00383
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00013	0.00140	-0.00187	0.00235	0.00271	-0.00383
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00014	0.00141	-0.00186	0.00235	0.00272	-0.00382
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00018	0.00144	-0.00185	0.00233	0.00273	-0.00382
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00052	0.00197	-0.00204	0.00231	0.00279	-0.00376

Table S18 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **GLY** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	0.473949	-0.642544	0.168595	0.078759	-1.297526	0.084204
	ES*	-0.000217	0.009365	-0.009147	0.004160	0.010813	0.000059
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000235	0.009367	-0.009133	0.004152	0.010835	0.000066
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000246	0.009371	-0.009125	0.004148	0.010849	0.000072
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000279	0.009410	-0.009131	0.004138	0.010877	0.000095
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000629	0.010303	-0.009674	0.004195	0.010852	-0.000080
O2	Single molecule	-0.941985	-0.476057	1.418042	-0.032654	0.424340	-0.553088
	ES*	0.001344	-0.000364	-0.000981	-0.008140	-0.018961	0.002897
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001327	-0.000361	-0.000966	-0.008148	-0.018940	0.002904
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001315	-0.000356	-0.000959	-0.008154	-0.018929	0.002909
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001259	-0.000301	-0.000958	-0.008178	-0.018915	0.002926
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000466	0.000797	-0.001263	-0.008257	-0.019339	0.003028
N1	Single molecule	0.069894	-0.024158	-0.045737	-0.068693	-0.032845	0.013102
	ES*	-0.002135	0.004494	-0.002359	0.000396	0.000618	-0.000547
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002153	0.004497	-0.002343	0.000389	0.000640	-0.000540
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002167	0.004500	-0.002333	0.000384	0.000654	-0.000535
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002210	0.004527	-0.002318	0.000374	0.000682	-0.000519
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002472	0.004877	-0.002405	0.000368	0.000723	-0.000439
C1	Single molecule	0.361013	-0.469707	0.108694	-0.180894	0.054343	-0.167893
	ES*	-0.002226	0.005211	-0.002984	-0.001709	-0.003190	0.004135
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002244	0.005213	-0.002969	-0.001717	-0.003168	0.004142
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002256	0.005217	-0.002961	-0.001722	-0.003156	0.004147
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002298	0.005255	-0.002957	-0.001738	-0.003134	0.004166
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002773	0.005963	-0.003189	-0.001780	-0.003151	0.004233
C2	Single molecule	-0.247094	0.053112	0.193983	0.211455	0.074060	-0.055756
	ES*	-0.000412	0.005111	-0.004699	0.000396	-0.000083	-0.000331
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000431	0.005114	-0.004683	0.000388	-0.000061	-0.000324
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000444	0.005118	-0.004674	0.000383	-0.000048	-0.000320
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000491	0.005150	-0.004659	0.000363	-0.000027	-0.000307
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000876	0.005639	-0.004763	0.000234	0.000048	-0.000245
H1	Single molecule	0.173749	0.218875	-0.392624	-0.032180	0.195893	0.101075
	ES*	-0.006747	-0.006856	0.013603	-0.004794	-0.011608	-0.000247
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.006767	-0.006852	0.013619	-0.004802	-0.011586	-0.000239
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.006780	-0.006849	0.013629	-0.004807	-0.011572	-0.000234
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.006826	-0.006822	0.013647	-0.004818	-0.011544	-0.000221
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.007098	-0.006499	0.013598	-0.004838	-0.011536	-0.000159

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H2	Single molecule	-0.120558	0.162948	-0.042390	-0.185005	-0.349797	-0.169841
	ES*	0.000905	-0.002684	0.001779	0.003406	0.019532	0.010657
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000886	-0.002681	0.001794	0.003399	0.019555	0.010664
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000874	-0.002678	0.001804	0.003394	0.019569	0.010669
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000835	-0.002655	0.001820	0.003386	0.019601	0.010688
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000615	-0.002322	0.001707	0.003395	0.019669	0.010807
H3	Single molecule	0.246990	-0.491000	0.244010	-0.077749	0.009650	0.120513
	ES*	0.005878	0.015612	-0.021490	0.006800	-0.007233	-0.005783
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005859	0.015615	-0.021474	0.006793	-0.007210	-0.005776
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005846	0.015619	-0.021465	0.006788	-0.007197	-0.005771
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005803	0.015647	-0.021451	0.006782	-0.007169	-0.005754
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005555	0.015962	-0.021517	0.006830	-0.007119	-0.005686
H4	Single molecule	0.202284	-0.436993	0.234709	-0.084184	0.021427	0.093549
	ES*	0.006258	0.005911	-0.012169	-0.001666	-0.003950	0.001568
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.006239	0.005914	-0.012153	-0.001674	-0.003928	0.001575
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.006226	0.005917	-0.012144	-0.001680	-0.003914	0.001579
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.006188	0.005934	-0.012123	-0.001709	-0.003888	0.001589
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005981	0.006162	-0.012143	-0.002018	-0.003743	0.001618
H5	Single molecule	-0.071321	0.144541	-0.073220	-0.132657	-0.283140	-0.159787
	ES*	0.000123	0.002396	-0.002518	0.003532	0.004047	-0.005745
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000104	0.002399	-0.002503	0.003525	0.004069	-0.005738
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000089	0.002404	-0.002493	0.003519	0.004080	-0.005733
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000025	0.002455	-0.002480	0.003500	0.004092	-0.005723
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000484	0.003247	-0.002764	0.003461	0.004181	-0.005641

Table S19 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **LAC** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.37435	0.26165	-0.14592	-0.05000	0.30373
	ES*	0.02717	-0.00148	-0.00242	-0.00499	0.00574
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.03029	-0.00146	-0.00244	-0.00497	0.00573
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.03031	-0.00145	-0.00246	-0.00496	0.00573
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.03036	-0.00141	-0.00249	-0.00494	0.00571
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.03056	-0.00135	-0.00256	-0.00485	0.00565
O2	Single molecule	-22.42856	-0.29674	0.14442	0.02043	0.33065
	ES*	0.07420	0.00859	-0.01225	-0.01335	0.02005
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07739	0.00861	-0.01227	-0.01331	0.02005
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07745	0.00862	-0.01229	-0.01329	0.02005
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07760	0.00864	-0.01232	-0.01324	0.02004
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07784	0.00858	-0.01249	-0.01312	0.02004
O3	Single molecule	-22.38160	-0.32430	-0.02556	0.13754	0.35319
	ES*	0.05469	0.03498	0.01170	-0.01080	0.03844
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05778	0.03498	0.01170	-0.01079	0.03843
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05778	0.03498	0.01170	-0.01078	0.03843
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05777	0.03498	0.01169	-0.01076	0.03842
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05776	0.03498	0.01166	-0.01068	0.03839
C1	Single molecule	-14.74433	-0.00816	0.04485	0.05246	0.06950
	ES*	0.04513	0.00884	-0.00468	-0.00609	0.01171
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04827	0.00886	-0.00470	-0.00607	0.01172
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04830	0.00887	-0.00471	-0.00606	0.01173
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04837	0.00889	-0.00474	-0.00603	0.01174
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04854	0.00890	-0.00483	-0.00593	0.01174
C2	Single molecule	-14.78244	0.01041	-0.03216	-0.05723	0.06647
	ES*	0.02617	0.01575	0.00257	-0.00332	0.01630
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02927	0.01576	0.00256	-0.00331	0.01631
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02927	0.01576	0.00256	-0.00331	0.01631
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02928	0.01578	0.00255	-0.00330	0.01632
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02930	0.01579	0.00250	-0.00325	0.01632
C3	Single molecule	-14.82899	-0.00321	-0.00983	0.01042	0.01468
	ES*	0.01965	0.00837	0.00289	-0.00103	0.00892
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02273	0.00837	0.00288	-0.00104	0.00891
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02272	0.00837	0.00288	-0.00104	0.00891
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02270	0.00836	0.00287	-0.00105	0.00890
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02256	0.00835	0.00278	-0.00107	0.00887

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H1	Single molecule	-1.01192	0.05958	0.00711	0.03959	0.07189
	ES*	0.00061	-0.01558	-0.01119	-0.01700	0.02563
	DS* (-4 < x_f, y_f, z_f < 5)	0.00379	-0.01556	-0.01122	-0.01697	0.02561
	DS* (-3 < x_f, y_f, z_f < 4)	0.00384	-0.01554	-0.01124	-0.01695	0.02560
	DS* (-2 < x_f, y_f, z_f < 3)	0.00397	-0.01550	-0.01129	-0.01692	0.02557
	DS* (-1 < x_f, y_f, z_f < 2)	0.00436	-0.01545	-0.01134	-0.01679	0.02548
H2	Single molecule	-1.08278	-0.00365	-0.01066	0.01476	0.01857
	ES*	-0.00084	0.01422	0.00529	0.00219	0.01533
	DS* (-4 < x_f, y_f, z_f < 5)	0.00225	0.01424	0.00528	0.00219	0.01534
	DS* (-3 < x_f, y_f, z_f < 4)	0.00225	0.01425	0.00527	0.00219	0.01535
	DS* (-2 < x_f, y_f, z_f < 3)	0.00225	0.01428	0.00527	0.00220	0.01538
	DS* (-1 < x_f, y_f, z_f < 2)	0.00231	0.01433	0.00525	0.00224	0.01543
H3	Single molecule	-0.98123	-0.02412	0.00180	0.00843	0.02562
	ES*	-0.00345	0.02647	0.01882	0.00606	0.03304
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00037	0.02647	0.01882	0.00607	0.03304
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00037	0.02647	0.01883	0.00608	0.03305
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00039	0.02647	0.01883	0.00609	0.03305
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00044	0.02649	0.01886	0.00613	0.03309
H4	Single molecule	-1.09022	0.00126	-0.03505	-0.01389	0.03772
	ES*	0.01551	0.00622	0.00372	-0.00203	0.00752
	DS* (-4 < x_f, y_f, z_f < 5)	0.01857	0.00622	0.00371	-0.00204	0.00753
	DS* (-3 < x_f, y_f, z_f < 4)	0.01854	0.00622	0.00371	-0.00204	0.00753
	DS* (-2 < x_f, y_f, z_f < 3)	0.01849	0.00623	0.00369	-0.00206	0.00753
	DS* (-1 < x_f, y_f, z_f < 2)	0.01823	0.00628	0.00358	-0.00205	0.00752
H5	Single molecule	-1.09038	0.01754	-0.00757	0.01664	0.02534
	ES*	0.00658	0.00697	0.00784	-0.00079	0.01052
	DS* (-4 < x_f, y_f, z_f < 5)	0.00968	0.00697	0.00784	-0.00081	0.01052
	DS* (-3 < x_f, y_f, z_f < 4)	0.00969	0.00696	0.00784	-0.00082	0.01052
	DS* (-2 < x_f, y_f, z_f < 3)	0.00970	0.00695	0.00784	-0.00084	0.01051
	DS* (-1 < x_f, y_f, z_f < 2)	0.00973	0.00689	0.00775	-0.00095	0.01041
H6	Single molecule	-1.10541	-0.01827	-0.01282	0.01536	0.02709
	ES*	0.03007	0.00685	-0.00101	0.00253	0.00737
	DS* (-4 < x_f, y_f, z_f < 5)	0.03314	0.00684	-0.00101	0.00252	0.00736
	DS* (-3 < x_f, y_f, z_f < 4)	0.03312	0.00683	-0.00102	0.00252	0.00735
	DS* (-2 < x_f, y_f, z_f < 3)	0.03309	0.00681	-0.00103	0.00251	0.00733
	DS* (-1 < x_f, y_f, z_f < 2)	0.03283	0.00677	-0.00112	0.00251	0.00731

Table S20 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **LAC** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.176027	-1306.087587	-1306.828767	-0.177811	-0.569160	-0.830242
	ES*	0.002578	-0.003413	0.000271	0.002697	0.004770	0.001040
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002579	-0.003412	0.000269	0.002699	0.004764	0.001043
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002579	-0.003411	0.000268	0.002701	0.004761	0.001044
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002580	-0.003409	0.000265	0.002704	0.004752	0.001049
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002602	-0.003429	0.000264	0.002696	0.004730	0.001057
O2	Single molecule	-1306.289899	-1306.108170	-1305.328541	0.226967	0.497356	0.836688
	ES*	0.004203	-0.002624	-0.003323	0.001806	0.001485	-0.006426
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004203	-0.002623	-0.003324	0.001809	0.001479	-0.006424
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004203	-0.002622	-0.003325	0.001810	0.001476	-0.006422
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004206	-0.002621	-0.003328	0.001814	0.001468	-0.006418
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004268	-0.002677	-0.003335	0.001849	0.001477	-0.006412
ATOM	**CALCULATION**	**XX**	**YY**	**ZZ**	**XY**	**XZ**	**YZ**
O3	Single molecule	-1306.045258	-1306.287172	-1305.982346	-0.494128	0.240946	-1.240779
	ES*	-0.007363	0.006479	-0.004888	-0.000970	0.011531	0.009281
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.007363	0.006480	-0.004890	-0.000967	0.011526	0.009283
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.007363	0.006481	-0.004890	-0.000966	0.011522	0.009285
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.007362	0.006482	-0.004893	-0.000962	0.011513	0.009289
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.007362	0.006488	-0.004898	-0.000931	0.011482	0.009303
C1	Single molecule	-534.065690	-534.481567	-534.358720	-0.145435	0.167194	0.197079
	ES*	0.000776	0.000142	-0.001032	0.003249	0.002625	-0.000219
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000776	0.000143	-0.001033	0.003251	0.002619	-0.000216
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000777	0.000144	-0.001034	0.003253	0.002616	-0.000214
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000778	0.000145	-0.001037	0.003256	0.002607	-0.000210
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000806	0.000124	-0.001044	0.003266	0.002594	-0.000203
C2	Single molecule	-533.768864	-533.836493	-533.918186	0.059850	0.067907	-0.153208
	ES*	-0.000829	0.002275	-0.001572	0.002936	0.002597	-0.000082
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000829	0.002276	-0.001574	0.002938	0.002591	-0.000080
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000829	0.002277	-0.001575	0.002940	0.002588	-0.000078
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000828	0.002278	-0.001577	0.002944	0.002579	-0.000074
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000827	0.002289	-0.001589	0.002958	0.002555	-0.000065
C3	Single molecule	-533.260257	-533.249187	-533.272189	-0.013831	0.006760	-0.001582
	ES*	-0.001276	0.000273	0.000915	0.003086	-0.000319	-0.000559
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001276	0.000274	0.000913	0.003088	-0.000324	-0.000557
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001276	0.000275	0.000912	0.003090	-0.000328	-0.000555
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001275	0.000276	0.000910	0.003094	-0.000337	-0.000551
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001271	0.000298	0.000884	0.003079	-0.000366	-0.000549

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H1	Single molecule	-2.072509	-1.826087	-1.988622	-0.060718	-0.214739	-0.063596
	ES*	-0.002549	-0.012614	-0.004886	0.007181	0.008390	0.004748
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002548	-0.012613	-0.004888	0.007183	0.008384	0.004751
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002548	-0.012612	-0.004889	0.007185	0.008381	0.004753
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002546	-0.012611	-0.004893	0.007188	0.008372	0.004757
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002504	-0.012642	-0.004904	0.007161	0.008346	0.004771
H2	Single molecule	-2.088463	-1.995976	-1.999055	-0.140595	0.153288	0.094231
	ES*	0.000929	0.000655	-0.002525	-0.001759	0.001489	0.001002
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000929	0.000656	-0.002527	-0.001756	0.001483	0.001005
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000929	0.000656	-0.002528	-0.001755	0.001479	0.001007
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000930	0.000658	-0.002530	-0.001751	0.001471	0.001011
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000918	0.000683	-0.002543	-0.001722	0.001450	0.001021
H3	Single molecule	-2.094732	-2.084609	-1.823889	-0.317777	-0.117214	-0.144308
	ES*	-0.008774	-0.000251	0.001422	-0.001372	0.000346	0.008327
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.008773	-0.000250	0.001421	-0.001369	0.000341	0.008330
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.008773	-0.000249	0.001420	-0.001368	0.000337	0.008332
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.008773	-0.000247	0.001418	-0.001364	0.000328	0.008336
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.008775	-0.000235	0.001407	-0.001326	0.000291	0.008350
H4	Single molecule	-2.009301	-2.089738	-2.257794	0.108112	0.155480	-0.214193
	ES*	-0.001284	0.001375	-0.000721	0.001770	-0.001165	0.001232
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001283	0.001376	-0.000723	0.001772	-0.001171	0.001235
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001283	0.001377	-0.000723	0.001774	-0.001174	0.001237
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001282	0.001378	-0.000726	0.001777	-0.001183	0.001241
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001271	0.001387	-0.000745	0.001748	-0.001201	0.001232
H5	Single molecule	-2.246801	-1.976495	-2.141425	-0.098398	-0.251182	-0.077914
	ES*	-0.001671	0.000728	0.000558	0.003716	-0.000015	0.000229
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001671	0.000729	0.000557	0.003719	-0.000020	0.000232
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001671	0.000729	0.000556	0.003720	-0.000024	0.000234
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001670	0.000731	0.000553	0.003723	-0.000033	0.000238
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001676	0.000776	0.000514	0.003699	-0.000072	0.000248
H6	Single molecule	-2.188107	-2.085304	-2.089368	-0.189367	0.192332	0.150903
	ES*	-0.001457	-0.002575	0.003806	0.002537	-0.000233	-0.000515
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001456	-0.002574	0.003805	0.002540	-0.000238	-0.000512
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001456	-0.002573	0.003804	0.002541	-0.000242	-0.000510
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001455	-0.002572	0.003802	0.002545	-0.000250	-0.000506
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001449	-0.002551	0.003774	0.002532	-0.000285	-0.000506

Table S21 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **LAC** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	0.282150	0.414809	-0.696960	-0.266717	-0.853739	-1.245363
	ES*	0.004149	-0.004837	0.000688	0.004045	0.007155	0.001560
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004150	-0.004836	0.000686	0.004049	0.007146	0.001564
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004150	-0.004835	0.000684	0.004051	0.007141	0.001566
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004152	-0.004832	0.000680	0.004056	0.007128	0.001573
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004184	-0.004861	0.000677	0.004043	0.007095	0.001585
O2	Single molecule	-0.571543	-0.298950	0.870493	0.340451	0.746034	1.255031
	ES*	0.007176	-0.003064	-0.004112	0.002710	0.002227	-0.009639
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.007176	-0.003062	-0.004114	0.002713	0.002219	-0.009636
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.007177	-0.003061	-0.004116	0.002716	0.002214	-0.009633
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.007180	-0.003060	-0.004121	0.002721	0.002202	-0.009627
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.007273	-0.003143	-0.004130	0.002773	0.002215	-0.009619
O3	Single molecule	0.089501	-0.273370	0.183869	-0.741192	0.361419	-1.861169
	ES*	-0.008159	0.012605	-0.004446	-0.001454	0.017297	0.013921
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.008158	0.012606	-0.004448	-0.001451	0.017289	0.013925
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.008158	0.012607	-0.004450	-0.001448	0.017283	0.013927
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.008157	0.012610	-0.004453	-0.001442	0.017270	0.013934
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.008157	0.012618	-0.004461	-0.001396	0.017222	0.013955
C1	Single molecule	0.354453	-0.269362	-0.085091	-0.218152	0.250791	0.295618
	ES*	0.001221	0.000270	-0.001490	0.004873	0.003937	-0.000328
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001221	0.000271	-0.001493	0.004877	0.003929	-0.000324
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001222	0.000272	-0.001494	0.004879	0.003924	-0.000321
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001224	0.000275	-0.001498	0.004885	0.003911	-0.000315
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001266	0.000243	-0.001510	0.004899	0.003890	-0.000305
C2	Single molecule	0.108476	0.007032	-0.115508	0.089776	0.101861	-0.229811
	ES*	-0.001181	0.003476	-0.002295	0.004404	0.003895	-0.000124
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001180	0.003477	-0.002297	0.004407	0.003887	-0.000120
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001180	0.003478	-0.002299	0.004410	0.003882	-0.000117
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001178	0.003481	-0.002302	0.004415	0.003869	-0.000111
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001177	0.003497	-0.002320	0.004437	0.003833	-0.000098
C3	Single molecule	0.000431	0.017036	-0.017467	-0.020747	0.010139	-0.002372
	ES*	-0.001870	0.000454	0.001416	0.004629	-0.000478	-0.000839
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001869	0.000455	0.001414	0.004633	-0.000487	-0.000835
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001869	0.000456	0.001413	0.004635	-0.000492	-0.000832
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001868	0.000459	0.001409	0.004640	-0.000505	-0.000826
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001862	0.000492	0.001371	0.004619	-0.000548	-0.000824

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H1	Single molecule	-0.165154	0.204479	-0.039325	-0.091078	-0.322108	-0.095394
	ES*	0.006202	-0.008896	0.002695	0.010771	0.012585	0.007122
	DS* (-4 < x_f, y_f, z_f < 5)	0.006202	-0.008895	0.002693	0.010774	0.012576	0.007126
	DS* (-3 < x_f, y_f, z_f < 4)	0.006203	-0.008894	0.002691	0.010777	0.012571	0.007129
	DS* (-2 < x_f, y_f, z_f < 3)	0.006206	-0.008891	0.002685	0.010782	0.012557	0.007136
	DS* (-1 < x_f, y_f, z_f < 2)	0.006269	-0.008938	0.002669	0.010741	0.012520	0.007156
H2	Single molecule	-0.090948	0.047783	0.043165	-0.210893	0.229931	0.141347
	ES*	0.001864	0.001453	-0.003317	-0.002638	0.002233	0.001503
	DS* (-4 < x_f, y_f, z_f < 5)	0.001865	0.001455	-0.003319	-0.002635	0.002225	0.001507
	DS* (-3 < x_f, y_f, z_f < 4)	0.001865	0.001456	-0.003321	-0.002632	0.002219	0.001510
	DS* (-2 < x_f, y_f, z_f < 3)	0.001866	0.001459	-0.003324	-0.002626	0.002206	0.001516
	DS* (-1 < x_f, y_f, z_f < 2)	0.001848	0.001496	-0.003343	-0.002584	0.002174	0.001532
H3	Single molecule	-0.140484	-0.125298	0.265782	-0.476665	-0.175821	-0.216463
	ES*	-0.009360	0.003425	0.005935	-0.002058	0.000519	0.012491
	DS* (-4 < x_f, y_f, z_f < 5)	-0.009359	0.003427	0.005933	-0.002054	0.000511	0.012495
	DS* (-3 < x_f, y_f, z_f < 4)	-0.009359	0.003428	0.005931	-0.002052	0.000506	0.012498
	DS* (-2 < x_f, y_f, z_f < 3)	-0.009358	0.003430	0.005928	-0.002046	0.000492	0.012504
	DS* (-1 < x_f, y_f, z_f < 2)	-0.009361	0.003449	0.005912	-0.001989	0.000437	0.012525
H4	Single molecule	0.164465	0.043810	-0.208275	0.162168	0.233220	-0.321290
	ES*	-0.001611	0.002378	-0.000767	0.002654	-0.001748	0.001848
	DS* (-4 < x_f, y_f, z_f < 5)	-0.001610	0.002379	-0.000769	0.002658	-0.001756	0.001852
	DS* (-3 < x_f, y_f, z_f < 4)	-0.001610	0.002380	-0.000770	0.002660	-0.001762	0.001855
	DS* (-2 < x_f, y_f, z_f < 3)	-0.001608	0.002382	-0.000774	0.002666	-0.001774	0.001861
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001592	0.002395	-0.000803	0.002623	-0.001801	0.001847
H5	Single molecule	-0.187840	0.217618	-0.029777	-0.147597	-0.376774	-0.116871
	ES*	-0.002314	0.001284	0.001030	0.005574	-0.000022	0.000344
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002314	0.001286	0.001028	0.005578	-0.000030	0.000348
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002313	0.001286	0.001027	0.005580	-0.000036	0.000350
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002312	0.001289	0.001023	0.005585	-0.000049	0.000357
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002321	0.001357	0.000964	0.005549	-0.000107	0.000372
H6	Single molecule	-0.100771	0.053434	0.047337	-0.284051	0.288498	0.226355
	ES*	-0.002072	-0.003750	0.005822	0.003806	-0.000349	-0.000772
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002072	-0.003748	0.005820	0.003810	-0.000357	-0.000768
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002071	-0.003747	0.005819	0.003812	-0.000363	-0.000766
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002070	-0.003745	0.005815	0.003817	-0.000376	-0.000759
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002061	-0.003714	0.005774	0.003799	-0.000427	-0.000759

Table S22 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **LDOPA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.45578	0.28915	0.05286	0.09986	0.31044
	ES*	0.15801	-0.01226	0.00264	-0.02825	0.03091
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.16435	-0.01221	0.00323	-0.02827	0.03096
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.16425	-0.01218	0.00325	-0.02827	0.03096
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.16322	-0.01198	0.00335	-0.02816	0.03078
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.15239	-0.00930	0.00388	-0.02666	0.02850
O2	Single molecule	-22.48075	-0.16628	-0.07663	0.25859	0.31685
	ES*	0.14707	-0.01260	0.00843	-0.03135	0.03483
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.15432	-0.01254	0.00901	-0.03140	0.03499
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.15445	-0.01248	0.00903	-0.03142	0.03499
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.15465	-0.01206	0.00905	-0.03147	0.03490
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.15912	-0.00712	0.00893	-0.03280	0.03473
O3	Single molecule	-22.44183	-0.17153	0.03759	-0.30158	0.34898
	ES*	0.01532	-0.00266	0.00635	0.01348	0.01514
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.00687	-0.00264	0.00693	0.01351	0.01541
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.00692	-0.00261	0.00693	0.01353	0.01542
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.00790	-0.00227	0.00672	0.01360	0.01534
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01640	0.00269	0.00547	0.01220	0.01364
O4	Single molecule	-22.44841	0.01186	0.29586	-0.17561	0.34426
	ES*	-0.01120	-0.00822	-0.02766	0.00235	0.02895
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.01778	-0.00821	-0.02712	0.00234	0.02843
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.01770	-0.00821	-0.02714	0.00234	0.02845
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.01671	-0.00818	-0.02731	0.00239	0.02860
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.00571	-0.00729	-0.02900	0.00293	0.03004
N1	Single molecule	-18.25937	-0.03566	-0.00816	0.03751	0.05239
	ES*	0.00789	-0.00439	0.00075	-0.01735	0.01791
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01428	-0.00437	0.00133	-0.01736	0.01795
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01420	-0.00434	0.00134	-0.01736	0.01795
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01366	-0.00420	0.00140	-0.01735	0.01790
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.00863	-0.00263	0.00174	-0.01726	0.01754
C1	Single molecule	-14.75258	0.01579	-0.00591	0.05337	0.05597
	ES*	0.11521	-0.01559	0.00554	-0.02889	0.03329
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.12195	-0.01554	0.00613	-0.02892	0.03340
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.12196	-0.01549	0.00614	-0.02894	0.03339
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.12157	-0.01520	0.00620	-0.02891	0.03324
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.11850	-0.01171	0.00643	-0.02885	0.03179

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C2	Single molecule	-14.73223	-0.04878	-0.01404	0.05210	0.07274
	ES*	0.03177	-0.01043	0.00373	-0.01980	0.02269
	DS* (-4 < x_f, y_f, z_f < 5)	0.03837	-0.01039	0.00431	-0.01983	0.02280
	DS* (-3 < x_f, y_f, z_f < 4)	0.03839	-0.01036	0.00432	-0.01984	0.02279
	DS* (-2 < x_f, y_f, z_f < 3)	0.03826	-0.01012	0.00436	-0.01986	0.02271
	DS* (-1 < x_f, y_f, z_f < 2)	0.03767	-0.00771	0.00447	-0.02023	0.02211
C3	Single molecule	-14.75732	-0.00651	0.01012	0.02184	0.02494
	ES*	0.00877	-0.01582	0.00258	-0.00877	0.01827
	DS* (-4 < x_f, y_f, z_f < 5)	0.00286	-0.01577	0.00317	-0.00880	0.01833
	DS* (-3 < x_f, y_f, z_f < 4)	0.00291	-0.01572	0.00319	-0.00882	0.01831
	DS* (-2 < x_f, y_f, z_f < 3)	0.00316	-0.01543	0.00321	-0.00887	0.01809
	DS* (-1 < x_f, y_f, z_f < 2)	0.00676	-0.01276	0.00323	-0.00952	0.01624
C4	Single molecule	-14.78922	-0.03377	0.01236	-0.04023	0.05396
	ES*	-0.01675	-0.00905	-0.00318	0.00009	0.00960
	DS* (-4 < x_f, y_f, z_f < 5)	-0.02282	-0.00902	-0.00260	0.00007	0.00939
	DS* (-3 < x_f, y_f, z_f < 4)	-0.02276	-0.00898	-0.00259	0.00005	0.00935
	DS* (-2 < x_f, y_f, z_f < 3)	-0.02230	-0.00876	-0.00263	0.00000	0.00914
	DS* (-1 < x_f, y_f, z_f < 2)	-0.01682	-0.00660	-0.00335	-0.00042	0.00742
C5	Single molecule	-14.81735	-0.04137	-0.01957	-0.01266	0.04748
	ES*	-0.00298	-0.00527	-0.00386	0.00072	0.00658
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01023	-0.00524	-0.00327	0.00072	0.00622
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01023	-0.00521	-0.00326	0.00071	0.00619
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00987	-0.00492	-0.00332	0.00071	0.00598
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00461	-0.00171	-0.00456	0.00048	0.00490
C6	Single molecule	-14.83888	-0.03080	-0.04438	0.02357	0.05894
	ES*	0.00137	-0.00412	-0.00164	0.00745	0.00867
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00601	-0.00410	-0.00106	0.00745	0.00857
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00597	-0.00407	-0.00106	0.00746	0.00856
	DS* (-2 < x_f, y_f, z_f < 3)	-0.00524	-0.00384	-0.00120	0.00747	0.00849
	DS* (-1 < x_f, y_f, z_f < 2)	0.00341	-0.00090	-0.00330	0.00682	0.00763
C7	Single molecule	-14.84521	0.02971	0.01222	0.04350	0.05407
	ES*	-0.01655	-0.00597	-0.01258	0.00335	0.01432
	DS* (-4 < x_f, y_f, z_f < 5)	-0.02292	-0.00596	-0.01202	0.00334	0.01382
	DS* (-3 < x_f, y_f, z_f < 4)	-0.02285	-0.00594	-0.01203	0.00333	0.01382
	DS* (-2 < x_f, y_f, z_f < 3)	-0.02205	-0.00584	-0.01216	0.00333	0.01390
	DS* (-1 < x_f, y_f, z_f < 2)	-0.01317	-0.00457	-0.01383	0.00314	0.01490
C8	Single molecule	-14.83031	0.02019	0.03050	0.00408	0.03681
	ES*	-0.05594	-0.00513	-0.01154	-0.00168	0.01274
	DS* (-4 < x_f, y_f, z_f < 5)	-0.04992	-0.00511	-0.01098	-0.00171	0.01224
	DS* (-3 < x_f, y_f, z_f < 4)	-0.04984	-0.00510	-0.01099	-0.00174	0.01224
	DS* (-2 < x_f, y_f, z_f < 3)	-0.04915	-0.00502	-0.01108	-0.00179	0.01229
	DS* (-1 < x_f, y_f, z_f < 2)	-0.04183	-0.00427	-0.01206	-0.00209	0.01297

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C9	Single molecule	-14.80906	-0.00040	0.02675	-0.01839	0.03246
	ES*	-0.05065	-0.00912	-0.00455	0.00208	0.01040
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.04444	-0.00908	-0.00398	0.00204	0.01013
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.04433	-0.00906	-0.00398	0.00202	0.01010
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.04365	-0.00892	-0.00404	0.00194	0.00998
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.03670	-0.00773	-0.00480	0.00132	0.00919
H1	Single molecule	-0.86705	-0.01201	0.00264	-0.01482	0.01925
	ES*	-0.03072	-0.00681	-0.00438	-0.02558	0.02683
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.02427	-0.00679	-0.00381	-0.02559	0.02674
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.02433	-0.00677	-0.00380	-0.02559	0.02674
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.02476	-0.00663	-0.00376	-0.02559	0.02670
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.02885	-0.00518	-0.00358	-0.02578	0.02654
H2	Single molecule	-0.87409	0.01373	0.01363	0.01479	0.02436
	ES*	0.00534	-0.00263	0.01427	-0.01292	0.01943
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01073	-0.00261	0.01486	-0.01292	0.01987
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01060	-0.00258	0.01489	-0.01292	0.01988
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.00977	-0.00243	0.01502	-0.01288	0.01993
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.00230	-0.00092	0.01584	-0.01254	0.02022
H3	Single molecule	-0.88237	0.00675	-0.02681	0.00665	0.02843
	ES*	0.01336	-0.00383	-0.01217	-0.01533	0.01994
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02048	-0.00381	-0.01159	-0.01533	0.01959
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02040	-0.00379	-0.01158	-0.01533	0.01958
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01977	-0.00369	-0.01153	-0.01530	0.01952
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01330	-0.00263	-0.01133	-0.01494	0.01894
H4	Single molecule	-1.01638	-0.02886	-0.00488	-0.03041	0.04220
	ES*	-0.00815	0.00851	0.01419	0.01902	0.02521
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.01723	0.00853	0.01480	0.01905	0.02558
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.01726	0.00858	0.01481	0.01908	0.02563
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.01673	0.00907	0.01468	0.01916	0.02578
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.01441	0.01552	0.01545	0.01685	0.02763
H5	Single molecule	-1.02872	0.01222	0.03455	-0.00474	0.03695
	ES*	-0.08148	-0.01438	-0.03637	-0.00513	0.03944
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.07597	-0.01438	-0.03584	-0.00515	0.03896
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.07594	-0.01439	-0.03586	-0.00516	0.03898
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.07514	-0.01439	-0.03600	-0.00510	0.03910
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.06530	-0.01383	-0.03711	-0.00420	0.03983
H6	Single molecule	-1.02387	-0.01208	-0.03817	0.00231	0.04010
	ES*	0.02040	-0.01517	0.00569	-0.01379	0.02127
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.02798	-0.01513	0.00626	-0.01383	0.02143
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.02804	-0.01509	0.00626	-0.01385	0.02142
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.02817	-0.01488	0.00626	-0.01391	0.02130
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.02990	-0.01267	0.00612	-0.01462	0.02029

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H7	Single molecule	-1.06011	-0.02743	0.00052	0.04887	0.05604
	ES*	-0.00891	-0.02469	0.00740	-0.00818	0.02704
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01462	-0.02464	0.00799	-0.00822	0.02717
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01446	-0.02458	0.00800	-0.00825	0.02714
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01366	-0.02428	0.00799	-0.00837	0.02690
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00481	-0.02168	0.00786	-0.00987	0.02508
H8	Single molecule	-1.03161	0.00652	0.03987	0.02183	0.04592
	ES*	0.02678	-0.01217	-0.00135	-0.01110	0.01653
	DS* (-4 < x_f, y_f, z_f < 5)	0.01986	-0.01212	-0.00074	-0.01113	0.01647
	DS* (-3 < x_f, y_f, z_f < 4)	0.01982	-0.01207	-0.00071	-0.01114	0.01644
	DS* (-2 < x_f, y_f, z_f < 3)	0.01965	-0.01172	-0.00063	-0.01115	0.01619
	DS* (-1 < x_f, y_f, z_f < 2)	0.01963	-0.00847	-0.00011	-0.01130	0.01412
H9	Single molecule	-1.05086	-0.00354	0.00623	0.00173	0.00738
	ES*	0.01209	-0.00635	-0.00532	-0.00813	0.01161
	DS* (-4 < x_f, y_f, z_f < 5)	0.00398	-0.00632	-0.00471	-0.00812	0.01132
	DS* (-3 < x_f, y_f, z_f < 4)	0.00389	-0.00627	-0.00469	-0.00812	0.01128
	DS* (-2 < x_f, y_f, z_f < 3)	0.00378	-0.00588	-0.00466	-0.00809	0.01103
	DS* (-1 < x_f, y_f, z_f < 2)	0.00476	-0.00162	-0.00488	-0.00819	0.00968
H10	Single molecule	-1.08195	-0.00624	-0.00859	0.00730	0.01289
	ES*	-0.07930	-0.00193	-0.01123	-0.00747	0.01363
	DS* (-4 < x_f, y_f, z_f < 5)	-0.07259	-0.00191	-0.01069	-0.00752	0.01321
	DS* (-3 < x_f, y_f, z_f < 4)	-0.07252	-0.00190	-0.01071	-0.00755	0.01324
	DS* (-2 < x_f, y_f, z_f < 3)	-0.07189	-0.00187	-0.01078	-0.00761	0.01333
	DS* (-1 < x_f, y_f, z_f < 2)	-0.06499	-0.00166	-0.01141	-0.00775	0.01389
H11	Single molecule	-1.06485	-0.01807	-0.00964	-0.00325	0.02074
	ES*	-0.06418	-0.01336	-0.00237	0.00415	0.01419
	DS* (-4 < x_f, y_f, z_f < 5)	-0.05708	-0.01333	-0.00181	0.00409	0.01406
	DS* (-3 < x_f, y_f, z_f < 4)	-0.05692	-0.01330	-0.00182	0.00406	0.01402
	DS* (-2 < x_f, y_f, z_f < 3)	-0.05612	-0.01316	-0.00186	0.00394	0.01386
	DS* (-1 < x_f, y_f, z_f < 2)	-0.04848	-0.01218	-0.00228	0.00299	0.01274

Table S23 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **LDOPA** molecule in the crystal from different calculations.
* Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.373610	-1306.118092	-1304.749096	-0.012937	-0.259498	-0.259318
	ES*	0.006095	-0.018672	0.009902	0.000615	0.000805	0.000720
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.006093	-0.018666	0.009898	0.000617	0.000810	0.000720
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.006087	-0.018660	0.009898	0.000619	0.000813	0.000721
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.006025	-0.018630	0.009930	0.000629	0.000842	0.000722
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005381	-0.018370	0.010314	0.000697	0.001370	0.000678
O2	Single molecule	-1305.427824	-1306.160626	-1305.655421	0.049126	0.866008	0.134533
	ES*	-0.003041	0.005223	-0.007687	-0.009644	-0.005333	-0.005918
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003043	0.005228	-0.007690	-0.009642	-0.005327	-0.005918
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003047	0.005232	-0.007691	-0.009640	-0.005321	-0.005917
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003063	0.005249	-0.007691	-0.009629	-0.005253	-0.005917
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002936	0.005396	-0.007965	-0.009548	-0.004256	-0.006055
O3	Single molecule	-1305.984466	-1306.548957	-1306.077093	-1.133750	-0.294407	0.638707
	ES*	-0.001821	0.002799	-0.001511	0.001489	0.003072	0.001596
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001823	0.002808	-0.001518	0.001492	0.003078	0.001602
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001818	0.002808	-0.001523	0.001498	0.003081	0.001606
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001755	0.002760	-0.001538	0.001560	0.003084	0.001621
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001416	0.003047	-0.002129	0.002924	0.003200	0.000772
O4	Single molecule	-1305.675633	-1306.325568	-1306.606489	-0.658418	-1.098481	-0.114856
	ES*	0.000539	-0.003572	0.000771	0.005672	0.002416	0.005493
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000538	-0.003565	0.000766	0.005675	0.002422	0.005499
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000542	-0.003564	0.000760	0.005675	0.002426	0.005503
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000601	-0.003592	0.000730	0.005671	0.002428	0.005512
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001331	-0.003979	0.000386	0.005608	0.002212	0.005494
N1	Single molecule	-863.209148	-863.265670	-863.218990	0.007119	-0.066282	-0.005708
	ES*	-0.001122	0.003264	-0.002535	-0.000557	0.001112	0.001141
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001123	0.003269	-0.002539	-0.000556	0.001117	0.001143
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001127	0.003274	-0.002541	-0.000553	0.001121	0.001145
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001157	0.003299	-0.002535	-0.000539	0.001136	0.001151
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001451	0.003484	-0.002426	-0.000416	0.001324	0.001178
C1	Single molecule	-533.818004	-534.358099	-533.941369	0.136381	-0.050678	-0.081868
	ES*	-0.000340	-0.000391	0.000407	-0.001050	-0.001271	0.001125
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000342	-0.000385	0.000403	-0.001048	-0.001266	0.001125
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000347	-0.000380	0.000403	-0.001046	-0.001261	0.001126
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000382	-0.000358	0.000415	-0.001033	-0.001219	0.001128
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000631	-0.000152	0.000458	-0.000943	-0.000582	0.001106

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C2	Single molecule	-534.043804	-533.812715	-533.982833	-0.041150	0.203339	0.010369
	ES*	0.003360	0.000297	-0.003748	-0.000715	-0.003136	0.000742
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003358	0.000303	-0.003751	-0.000713	-0.003130	0.000744
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003355	0.000307	-0.003753	-0.000711	-0.003126	0.000746
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003340	0.000324	-0.003754	-0.000696	-0.003100	0.000751
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003266	0.000451	-0.003808	-0.000582	-0.002785	0.000791
C3	Single molecule	-533.603826	-533.608983	-533.622808	0.006297	-0.010621	-0.009340
	ES*	0.003452	-0.000940	-0.002633	-0.000266	-0.004269	0.002638
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003450	-0.000933	-0.002638	-0.000264	-0.004264	0.002640
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003449	-0.000929	-0.002641	-0.000261	-0.004259	0.002642
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003455	-0.000923	-0.002652	-0.000232	-0.004233	0.002650
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003602	-0.000865	-0.002858	-0.000005	-0.004004	0.002786
C4	Single molecule	-534.618416	-534.552644	-534.555105	0.172592	0.078329	-0.102087
	ES*	0.001104	-0.000949	-0.000206	0.000081	-0.003230	0.001688
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001103	-0.000942	-0.000211	0.000083	-0.003225	0.001691
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001103	-0.000939	-0.000214	0.000087	-0.003221	0.001694
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001123	-0.000947	-0.000227	0.000112	-0.003205	0.001703
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001388	-0.001143	-0.000296	0.000405	-0.003154	0.001856
C5	Single molecule	-534.194939	-534.151900	-534.051716	0.131080	0.117245	-0.118758
	ES*	0.000187	0.001685	-0.001944	-0.000188	-0.001429	-0.001546
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000185	0.001693	-0.001949	-0.000185	-0.001423	-0.001542
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000186	0.001695	-0.001953	-0.000180	-0.001420	-0.001539
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000209	0.001682	-0.001963	-0.000135	-0.001408	-0.001527
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000405	0.001284	-0.001758	0.000581	-0.001440	-0.001432
C6	Single molecule	-534.565620	-534.514935	-534.460088	0.157455	0.110512	-0.099249
	ES*	-0.000946	0.003923	-0.003218	0.002029	0.000932	-0.000268
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000948	0.003931	-0.003224	0.002031	0.000938	-0.000263
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000945	0.003932	-0.003229	0.002035	0.000942	-0.000260
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000900	0.003901	-0.003242	0.002071	0.000948	-0.000248
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000336	0.003279	-0.003182	0.002730	0.000927	-0.000527
C7	Single molecule	-534.557484	-534.524840	-534.458548	0.156022	0.117266	-0.096428
	ES*	-0.002192	0.002643	-0.000781	0.002528	0.002368	0.002939
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002193	0.002650	-0.000787	0.002530	0.002374	0.002945
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002190	0.002652	-0.000791	0.002532	0.002378	0.002948
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002145	0.002626	-0.000811	0.002541	0.002383	0.002957
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001558	0.002171	-0.000942	0.002632	0.002267	0.002883
C8	Single molecule	-534.199140	-534.133152	-534.055283	0.137263	0.100467	-0.122840
	ES*	-0.002316	-0.000529	0.002659	0.001394	0.000558	0.002529
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002318	-0.000523	0.002654	0.001396	0.000564	0.002533
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002316	-0.000521	0.002651	0.001398	0.000568	0.002536
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002283	-0.000536	0.002633	0.001401	0.000577	0.002544
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001858	-0.000835	0.002507	0.001404	0.000522	0.002562

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C9	Single molecule	-534.157652	-534.145892	-534.073941	0.160141	0.135874	-0.070822
	ES*	-0.000990	-0.000791	0.001607	0.001501	-0.001957	0.001691
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000991	-0.000785	0.001603	0.001503	-0.001951	0.001694
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000990	-0.000783	0.001600	0.001505	-0.001947	0.001697
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000963	-0.000794	0.001584	0.001514	-0.001934	0.001703
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000597	-0.001026	0.001451	0.001600	-0.001921	0.001775
H1	Single molecule	-1.817213	-1.743818	-2.241671	-0.011946	-0.192606	-0.028622
	ES*	-0.008540	-0.008301	0.008144	-0.000522	0.003551	0.006318
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.008541	-0.008296	0.008140	-0.000521	0.003556	0.006321
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.008544	-0.008291	0.008138	-0.000518	0.003560	0.006324
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.008568	-0.008271	0.008141	-0.000503	0.003571	0.006331
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.008811	-0.008118	0.008232	-0.000363	0.003691	0.006356
H2	Single molecule	-1.882834	-2.179467	-1.745582	-0.242676	-0.033112	-0.067610
	ES*	-0.004769	0.010284	-0.010929	0.003662	0.000452	0.004881
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.004771	0.010290	-0.010934	0.003664	0.000458	0.004884
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.004775	0.010297	-0.010936	0.003667	0.000461	0.004886
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.004816	0.010331	-0.010929	0.003685	0.000474	0.004892
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.005224	0.010571	-0.010762	0.003841	0.000646	0.004922
H3	Single molecule	-2.002960	-2.046390	-1.749653	0.284197	-0.062018	0.074404
	ES*	-0.005591	0.010921	-0.010863	-0.003199	0.001359	-0.003994
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005592	0.010926	-0.010866	-0.003197	0.001365	-0.003992
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005596	0.010931	-0.010867	-0.003195	0.001368	-0.003990
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005631	0.010956	-0.010857	-0.003186	0.001381	-0.003985
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006006	0.011164	-0.010690	-0.003109	0.001572	-0.003970
H4	Single molecule	-2.153445	-1.997528	-1.911028	-0.275875	-0.198552	-0.123238
	ES*	0.005169	-0.002816	-0.014020	0.006344	0.007107	0.003412
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005167	-0.002807	-0.014027	0.006347	0.007112	0.003418
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005171	-0.002806	-0.014032	0.006356	0.007116	0.003422
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005212	-0.002836	-0.014043	0.006458	0.007120	0.003439
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004322	-0.001677	-0.014233	0.008063	0.007796	0.002083
H5	Single molecule	-1.937945	-2.261489	-1.857820	-0.268809	-0.099100	-0.140966
	ES*	-0.005367	0.007095	-0.008888	0.001576	0.003815	0.002559
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005368	0.007102	-0.008892	0.001579	0.003820	0.002566
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005365	0.007104	-0.008898	0.001579	0.003825	0.002570
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005313	0.007087	-0.008933	0.001573	0.003829	0.002579
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.004675	0.006835	-0.009319	0.001449	0.003613	0.002584
H6	Single molecule	-2.035771	-2.251630	-1.899871	-0.234556	-0.040572	-0.081002
	ES*	0.008207	-0.002857	-0.006013	0.001387	-0.003707	-0.002536
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.008205	-0.002852	-0.006016	0.001389	-0.003702	-0.002533
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.008203	-0.002848	-0.006018	0.001391	-0.003697	-0.002532
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.008198	-0.002838	-0.006023	0.001398	-0.003672	-0.002528
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.008246	-0.002766	-0.006143	0.001438	-0.003397	-0.002504

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-2.166923	-1.891842	-2.158260	-0.025626	0.274412	0.021929
	ES*	0.000732	0.001202	-0.004301	0.000169	-0.002933	0.002729
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000730	0.001208	-0.004306	0.000171	-0.002928	0.002731
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000730	0.001212	-0.004309	0.000174	-0.002923	0.002732
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000755	0.001209	-0.004332	0.000198	-0.002891	0.002739
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001178	0.001256	-0.004802	0.000419	-0.002623	0.002847
H8	Single molecule	-2.059639	-2.248022	-1.908688	-0.242411	-0.053531	-0.080190
	ES*	0.008043	-0.005727	-0.002910	0.000194	-0.006074	0.002779
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.008041	-0.005719	-0.002916	0.000196	-0.006068	0.002781
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.008038	-0.005714	-0.002919	0.000201	-0.006064	0.002783
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.008028	-0.005697	-0.002925	0.000245	-0.006037	0.002793
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.008031	-0.005585	-0.003039	0.000499	-0.005773	0.003006
H9	Single molecule	-2.143705	-2.116914	-1.943058	-0.226923	-0.086447	-0.061966
	ES*	0.000675	-0.000450	-0.000807	-0.001713	-0.001820	-0.007357
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000673	-0.000442	-0.000813	-0.001710	-0.001815	-0.007353
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000672	-0.000438	-0.000817	-0.001703	-0.001811	-0.007350
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000675	-0.000435	-0.000823	-0.001631	-0.001800	-0.007335
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000343	-0.000361	-0.000542	-0.000712	-0.002003	-0.007233
H10	Single molecule	-2.163256	-2.091862	-1.947997	-0.228081	-0.098513	-0.071266
	ES*	-0.003914	-0.004246	0.006750	0.000278	-0.000016	0.001450
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003916	-0.004241	0.006746	0.000280	-0.000010	0.001455
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003914	-0.004239	0.006742	0.000281	-0.000006	0.001458
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003883	-0.004251	0.006723	0.000280	0.000004	0.001465
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003487	-0.004459	0.006536	0.000216	-0.000059	0.001482
H11	Single molecule	-1.933839	-2.151057	-2.118179	-0.083427	0.061240	0.228490
	ES*	-0.001850	-0.001068	0.002354	0.000066	-0.002958	0.000121
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001852	-0.001063	0.002351	0.000068	-0.002953	0.000124
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001851	-0.001061	0.002348	0.000070	-0.002948	0.000126
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001825	-0.001069	0.002330	0.000074	-0.002934	0.000131
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001452	-0.001222	0.002110	0.000099	-0.002912	0.000183

Table S24 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **LDOPA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-0.940016	-0.556739	1.496755	-0.019406	-0.389247	-0.388977
	ES*	0.010480	-0.026670	0.016190	0.000923	0.001207	0.001079
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.010477	-0.026661	0.016184	0.000926	0.001215	0.001080
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.010468	-0.026653	0.016185	0.000928	0.001220	0.001081
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.010376	-0.026608	0.016232	0.000944	0.001262	0.001083
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.009410	-0.026218	0.016808	0.001046	0.002055	0.001018
O2	Single molecule	0.480199	-0.619004	0.138804	0.073689	1.299013	0.201800
	ES*	-0.001809	0.010587	-0.008778	-0.014466	-0.007999	-0.008876
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001812	0.010595	-0.008783	-0.014463	-0.007991	-0.008876
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001818	0.010601	-0.008783	-0.014460	-0.007981	-0.008876
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001842	0.010626	-0.008784	-0.014444	-0.007880	-0.008875
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001651	0.010846	-0.009195	-0.014322	-0.006384	-0.009083
O3	Single molecule	0.328559	-0.518177	0.189618	-1.700624	-0.441611	0.958061
	ES*	-0.002465	0.004465	-0.002000	0.002234	0.004608	0.002394
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002467	0.004478	-0.002010	0.002238	0.004616	0.002403
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002460	0.004478	-0.002018	0.002247	0.004622	0.002409
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002366	0.004407	-0.002041	0.002340	0.004626	0.002431
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001875	0.004819	-0.002945	0.004386	0.004799	0.001157
O4	Single molecule	0.790395	-0.184507	-0.605888	-0.987627	-1.647722	-0.172284
	ES*	0.001940	-0.004228	0.002288	0.008508	0.003624	0.008239
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001938	-0.004217	0.002279	0.008512	0.003633	0.008248
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001944	-0.004215	0.002271	0.008513	0.003639	0.008254
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002032	-0.004258	0.002226	0.008507	0.003642	0.008268
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003128	-0.004837	0.001709	0.008413	0.003318	0.008241
N1	Single molecule	0.033182	-0.051601	0.018419	0.010679	-0.099423	-0.008562
	ES*	-0.001486	0.005092	-0.003606	-0.000836	0.001668	0.001711
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001488	0.005101	-0.003612	-0.000833	0.001676	0.001715
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001493	0.005108	-0.003615	-0.000830	0.001681	0.001718
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001539	0.005145	-0.003606	-0.000808	0.001703	0.001727
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001980	0.005423	-0.003443	-0.000623	0.001986	0.001767
C1	Single molecule	0.331730	-0.478413	0.146683	0.204572	-0.076017	-0.122802
	ES*	-0.000348	-0.000424	0.000772	-0.001575	-0.001907	0.001687
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000351	-0.000415	0.000767	-0.001573	-0.001899	0.001688
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000358	-0.000408	0.000766	-0.001569	-0.001892	0.001689
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000410	-0.000374	0.000785	-0.001549	-0.001829	0.001693
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000784	-0.000065	0.000849	-0.001414	-0.000873	0.001659

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C2	Single molecule	-0.146030	0.200604	-0.054574	-0.061726	0.305008	0.015554
	ES*	0.005085	0.000491	-0.005576	-0.001073	-0.004703	0.001114
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005082	0.000500	-0.005582	-0.001070	-0.004695	0.001117
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005078	0.000506	-0.005584	-0.001066	-0.004689	0.001119
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005055	0.000531	-0.005585	-0.001043	-0.004649	0.001126
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004945	0.000722	-0.005666	-0.000873	-0.004177	0.001186
C3	Single molecule	0.012069	0.004334	-0.016403	0.009446	-0.015932	-0.014010
	ES*	0.005239	-0.001349	-0.003890	-0.000400	-0.006404	0.003957
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005236	-0.001339	-0.003897	-0.000396	-0.006395	0.003960
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005234	-0.001333	-0.003901	-0.000391	-0.006388	0.003963
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005243	-0.001324	-0.003918	-0.000348	-0.006350	0.003974
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005464	-0.001238	-0.004226	-0.000008	-0.006006	0.004179
C4	Single molecule	-0.064542	0.034117	0.030425	0.258888	0.117494	-0.153131
	ES*	0.001682	-0.001398	-0.000284	0.000121	-0.004845	0.002532
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001679	-0.001388	-0.000291	0.000125	-0.004837	0.002537
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001680	-0.001383	-0.000296	0.000130	-0.004831	0.002541
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001710	-0.001395	-0.000315	0.000169	-0.004807	0.002554
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002107	-0.001689	-0.000418	0.000608	-0.004731	0.002783
C5	Single molecule	-0.093131	-0.028573	0.121704	0.196619	0.175868	-0.178137
	ES*	0.000316	0.002563	-0.002880	-0.000281	-0.002143	-0.002319
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000314	0.002575	-0.002888	-0.000278	-0.002135	-0.002313
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000315	0.002579	-0.002894	-0.000270	-0.002129	-0.002308
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000350	0.002559	-0.002908	-0.000202	-0.002112	-0.002290
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000642	0.001960	-0.002602	0.000872	-0.002160	-0.002148
C6	Single molecule	-0.078109	-0.002081	0.080190	0.236182	0.165769	-0.148873
	ES*	-0.001299	0.006005	-0.004707	0.003043	0.001399	-0.000402
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001301	0.006017	-0.004716	0.003047	0.001407	-0.000395
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001297	0.006019	-0.004722	0.003053	0.001413	-0.000390
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001229	0.005972	-0.004743	0.003107	0.001423	-0.000372
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000385	0.005038	-0.004654	0.004094	0.001391	-0.000790
C7	Single molecule	-0.065789	-0.016825	0.082614	0.234033	0.175899	-0.144642
	ES*	-0.003122	0.004130	-0.001007	0.003792	0.003552	0.004409
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003125	0.004140	-0.001015	0.003796	0.003561	0.004417
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003120	0.004142	-0.001022	0.003798	0.003567	0.004422
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003053	0.004104	-0.001051	0.003811	0.003575	0.004436
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002173	0.003421	-0.001249	0.003948	0.003401	0.004324
C8	Single molecule	-0.104923	-0.005940	0.110863	0.205894	0.150700	-0.184260
	ES*	-0.003381	-0.000700	0.004081	0.002091	0.000838	0.003793
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003384	-0.000691	0.004075	0.002095	0.000846	0.003800
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003381	-0.000688	0.004069	0.002097	0.000852	0.003804
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003331	-0.000711	0.004043	0.002102	0.000865	0.003815
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002694	-0.001160	0.003854	0.002106	0.000782	0.003843

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C9	Single molecule	-0.047735	-0.030095	0.077830	0.240212	0.203811	-0.106234
	ES*	-0.001398	-0.001099	0.002497	0.002251	-0.002935	0.002536
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001400	-0.001091	0.002491	0.002255	-0.002926	0.002541
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001399	-0.001087	0.002486	0.002258	-0.002920	0.002545
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001358	-0.001104	0.002462	0.002272	-0.002901	0.002555
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000809	-0.001453	0.002262	0.002400	-0.002882	0.002663
H1	Single molecule	0.175532	0.285624	-0.461155	-0.017919	-0.288909	-0.042933
	ES*	-0.008461	-0.008103	0.016564	-0.000784	0.005326	0.009476
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.008463	-0.008095	0.016558	-0.000781	0.005334	0.009482
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.008467	-0.008088	0.016556	-0.000777	0.005339	0.009485
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.008503	-0.008057	0.016560	-0.000754	0.005357	0.009496
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.008867	-0.007829	0.016696	-0.000544	0.005536	0.009534
H2	Single molecule	0.079691	-0.365259	0.285568	-0.364014	-0.049669	-0.101415
	ES*	-0.004446	0.018133	-0.013687	0.005493	0.000679	0.007322
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.004449	0.018143	-0.013694	0.005496	0.000686	0.007326
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.004455	0.018152	-0.013697	0.005500	0.000691	0.007329
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.004517	0.018203	-0.013686	0.005527	0.000711	0.007338
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.005128	0.018564	-0.013435	0.005761	0.000968	0.007382
H3	Single molecule	-0.104939	-0.170083	0.275022	0.426295	-0.093027	0.111606
	ES*	-0.005620	0.019147	-0.013528	-0.004798	0.002039	-0.005992
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005622	0.019155	-0.013533	-0.004795	0.002047	-0.005988
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005628	0.019162	-0.013534	-0.004793	0.002052	-0.005985
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005681	0.019200	-0.013519	-0.004779	0.002072	-0.005978
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006243	0.019512	-0.013268	-0.004664	0.002358	-0.005956
H4	Single molecule	-0.199166	0.034708	0.164458	-0.413813	-0.297828	-0.184858
	ES*	0.013587	0.001609	-0.015196	0.009516	0.010660	0.005119
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.013585	0.001622	-0.015207	0.009520	0.010668	0.005127
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.013589	0.001625	-0.015214	0.009535	0.010673	0.005134
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.013651	0.001580	-0.015231	0.009687	0.010681	0.005159
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.012277	0.003279	-0.015555	0.012094	0.011694	0.003125
H5	Single molecule	0.121710	-0.363607	0.241897	-0.403213	-0.148649	-0.211448
	ES*	-0.004471	0.014223	-0.009752	0.002365	0.005722	0.003839
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.004473	0.014232	-0.009759	0.002368	0.005731	0.003848
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.004468	0.014235	-0.009767	0.002369	0.005737	0.003854
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.004390	0.014209	-0.009819	0.002359	0.005743	0.003868
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003433	0.013832	-0.010399	0.002174	0.005419	0.003876
H6	Single molecule	0.039979	-0.283809	0.243830	-0.351834	-0.060857	-0.121504
	ES*	0.012642	-0.003953	-0.008688	0.002081	-0.005561	-0.003803
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.012639	-0.003946	-0.008693	0.002084	-0.005552	-0.003800
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.012636	-0.003941	-0.008695	0.002087	-0.005546	-0.003798
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.012628	-0.003925	-0.008703	0.002098	-0.005508	-0.003792
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.012701	-0.003817	-0.008883	0.002158	-0.005096	-0.003755

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-0.141872	0.270749	-0.128877	-0.038440	0.411619	0.032894
	ES*	0.002282	0.002987	-0.005268	0.000253	-0.004400	0.004094
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002279	0.002996	-0.005275	0.000256	-0.004392	0.004096
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002279	0.003001	-0.005280	0.000261	-0.004384	0.004098
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002317	0.002998	-0.005314	0.000297	-0.004337	0.004108
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002951	0.003068	-0.006019	0.000628	-0.003935	0.004270
H8	Single molecule	0.018716	-0.263858	0.245142	-0.363616	-0.080296	-0.120285
	ES*	0.012361	-0.008293	-0.004068	0.000291	-0.009111	0.004169
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.012358	-0.008282	-0.004076	0.000294	-0.009103	0.004172
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.012355	-0.008274	-0.004081	0.000301	-0.009096	0.004175
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.012340	-0.008249	-0.004091	0.000367	-0.009056	0.004190
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.012343	-0.008082	-0.004262	0.000748	-0.008660	0.004509
H9	Single molecule	-0.113719	-0.073533	0.187252	-0.340385	-0.129670	-0.092949
	ES*	0.001303	-0.000384	-0.000919	-0.002569	-0.002730	-0.011036
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001301	-0.000372	-0.000929	-0.002565	-0.002722	-0.011030
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001300	-0.000365	-0.000935	-0.002554	-0.002717	-0.011025
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001305	-0.000362	-0.000943	-0.002447	-0.002699	-0.011003
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000795	-0.000262	-0.000533	-0.001068	-0.003005	-0.010849
H10	Single molecule	-0.143326	-0.036236	0.179562	-0.342122	-0.147770	-0.106899
	ES*	-0.005166	-0.005664	0.010830	0.000417	-0.000024	0.002175
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005168	-0.005656	0.010824	0.000420	-0.000015	0.002182
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005166	-0.005653	0.010819	0.000422	-0.000008	0.002187
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005119	-0.005671	0.010789	0.000419	0.000005	0.002197
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.004525	-0.005984	0.010509	0.000325	-0.000088	0.002223
H11	Single molecule	0.200780	-0.125048	-0.075731	-0.125141	0.091860	0.342736
	ES*	-0.002493	-0.001320	0.003814	0.000099	-0.004437	0.000182
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002496	-0.001313	0.003808	0.000102	-0.004429	0.000186
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002495	-0.001310	0.003804	0.000104	-0.004422	0.000189
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002455	-0.001322	0.003777	0.000111	-0.004401	0.000197
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001896	-0.001551	0.003447	0.000148	-0.004368	0.000275

Table S25 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **PARA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.42223	-0.27038	0.07899	0.18437	0.33666
	ES*	0.05919	0.01149	0.00153	-0.01927	0.02249
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07623	0.01149	0.00156	-0.01920	0.02243
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07627	0.01148	0.00158	-0.01916	0.02239
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07639	0.01147	0.00164	-0.01905	0.02230
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07726	0.01136	0.00176	-0.01845	0.02174
O2	Single molecule	-22.42733	-0.21779	0.02268	0.25519	0.33626
	ES*	0.08314	0.00185	-0.00583	-0.02397	0.02474
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.10010	0.00184	-0.00582	-0.02396	0.02473
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.10010	0.00184	-0.00581	-0.02396	0.02472
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.10009	0.00183	-0.00580	-0.02394	0.02470
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.10001	0.00178	-0.00573	-0.02390	0.02464
N1	Single molecule	-18.42788	-0.00580	-0.00835	0.01466	0.01784
	ES*	0.02107	0.00697	-0.00491	-0.01381	0.01623
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.03809	0.00697	-0.00490	-0.01379	0.01621
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.03813	0.00697	-0.00490	-0.01377	0.01619
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.03823	0.00697	-0.00489	-0.01373	0.01615
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.03852	0.00694	-0.00487	-0.01359	0.01602
C1	Single molecule	-14.81784	-0.05436	0.04137	-0.01420	0.06978
	ES*	0.03369	0.00468	-0.00606	-0.00850	0.01144
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05073	0.00468	-0.00605	-0.00847	0.01141
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05078	0.00467	-0.00604	-0.00844	0.01139
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05089	0.00467	-0.00603	-0.00838	0.01133
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05119	0.00465	-0.00600	-0.00820	0.01117
C2	Single molecule	-14.85805	0.01086	0.01364	-0.01643	0.02396
	ES*	0.04690	-0.00067	-0.00519	-0.00485	0.00713
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06389	-0.00068	-0.00517	-0.00482	0.00710
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06390	-0.00068	-0.00516	-0.00479	0.00707
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06394	-0.00069	-0.00513	-0.00474	0.00702
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06396	-0.00072	-0.00506	-0.00453	0.00683
C3	Single molecule	-14.85201	0.02632	0.00014	-0.01024	0.02824
	ES*	0.05421	0.00070	-0.00722	-0.00131	0.00737
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07119	0.00069	-0.00720	-0.00126	0.00734
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07120	0.00069	-0.00718	-0.00123	0.00732
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07122	0.00068	-0.00715	-0.00116	0.00727
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07127	0.00064	-0.00705	-0.00085	0.00713

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C4	Single molecule	-14.81935	0.02917	-0.03184	0.02465	0.04972
	ES*	0.05347	0.00469	-0.00208	-0.00648	0.00826
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07051	0.00468	-0.00206	-0.00642	0.00821
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07057	0.00468	-0.00204	-0.00639	0.00818
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07070	0.00467	-0.00200	-0.00630	0.00809
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07140	0.00465	-0.00195	-0.00583	0.00771
C5	Single molecule	-14.82579	-0.00652	-0.02173	0.03011	0.03770
	ES*	0.03794	0.00328	-0.00134	-0.00440	0.00565
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05505	0.00327	-0.00132	-0.00435	0.00560
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05516	0.00327	-0.00131	-0.00431	0.00557
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05541	0.00327	-0.00128	-0.00422	0.00549
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.05666	0.00330	-0.00133	-0.00371	0.00514
C6	Single molecule	-14.83118	-0.02426	-0.00366	0.02195	0.03292
	ES*	0.02723	0.00586	-0.00571	-0.00462	0.00940
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04433	0.00586	-0.00570	-0.00457	0.00936
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04441	0.00586	-0.00569	-0.00454	0.00935
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04464	0.00586	-0.00567	-0.00447	0.00930
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04542	0.00585	-0.00571	-0.00417	0.00918
C7	Single molecule	-14.74815	-0.02466	0.00656	0.02090	0.03298
	ES*	0.04561	0.00499	-0.00432	-0.01395	0.01543
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06259	0.00499	-0.00432	-0.01393	0.01541
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06261	0.00499	-0.00431	-0.01392	0.01541
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06264	0.00499	-0.00431	-0.01390	0.01538
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06274	0.00496	-0.00427	-0.01383	0.01530
C8	Single molecule	-14.82076	0.01897	-0.01980	0.01188	0.02988
	ES*	0.03022	0.00289	-0.00448	-0.00811	0.00970
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04720	0.00289	-0.00448	-0.00810	0.00970
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04721	0.00290	-0.00448	-0.00810	0.00970
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04724	0.00290	-0.00449	-0.00809	0.00969
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04739	0.00289	-0.00450	-0.00806	0.00967
H1	Single molecule	-1.12603	0.00833	-0.01077	0.01915	0.02350
	ES*	0.04849	-0.00634	-0.00186	-0.00607	0.00897
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06545	-0.00634	-0.00185	-0.00604	0.00895
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06545	-0.00635	-0.00184	-0.00603	0.00894
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06544	-0.00636	-0.00181	-0.00598	0.00892
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06526	-0.00641	-0.00173	-0.00583	0.00883
H2	Single molecule	-1.11243	-0.01286	0.00692	0.00528	0.01553
	ES*	0.05156	-0.00247	-0.01073	0.00347	0.01155
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.06850	-0.00247	-0.01071	0.00352	0.01154
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.06847	-0.00248	-0.01069	0.00354	0.01153
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.06841	-0.00250	-0.01065	0.00362	0.01152
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.06809	-0.00258	-0.01051	0.00392	0.01151

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H3	Single molecule	-1.07542	0.00428	0.00535	-0.00288	0.00743
	ES*	0.03383	-0.00021	-0.00062	0.00049	0.00082
	DS* (-4 < x_f, y_f, z_f < 5)	0.05101	-0.00021	-0.00060	0.00056	0.00085
	DS* (-3 < x_f, y_f, z_f < 4)	0.05116	-0.00021	-0.00059	0.00060	0.00086
	DS* (-2 < x_f, y_f, z_f < 3)	0.05153	-0.00021	-0.00056	0.00070	0.00092
	DS* (-1 < x_f, y_f, z_f < 2)	0.05391	-0.00015	-0.00063	0.00156	0.00169
H4	Single molecule	-1.07651	0.00073	0.00352	-0.00252	0.00439
	ES*	0.01126	0.00870	-0.00936	-0.00062	0.01280
	DS* (-4 < x_f, y_f, z_f < 5)	0.02839	0.00870	-0.00935	-0.00058	0.01279
	DS* (-3 < x_f, y_f, z_f < 4)	0.02851	0.00871	-0.00935	-0.00055	0.01279
	DS* (-2 < x_f, y_f, z_f < 3)	0.02879	0.00871	-0.00934	-0.00047	0.01278
	DS* (-1 < x_f, y_f, z_f < 2)	0.02986	0.00870	-0.00939	-0.00015	0.01280
H5	Single molecule	-1.01889	-0.02141	-0.01405	0.04849	0.05484
	ES*	0.01198	0.00282	0.00787	-0.02990	0.03105
	DS* (-4 < x_f, y_f, z_f < 5)	0.02911	0.00282	0.00790	-0.02983	0.03099
	DS* (-3 < x_f, y_f, z_f < 4)	0.02922	0.00281	0.00792	-0.02978	0.03094
	DS* (-2 < x_f, y_f, z_f < 3)	0.02951	0.00281	0.00797	-0.02966	0.03084
	DS* (-1 < x_f, y_f, z_f < 2)	0.03154	0.00267	0.00808	-0.02882	0.03005
H6	Single molecule	-1.00100	-0.02019	0.00404	0.00036	0.02059
	ES*	-0.01717	0.01837	-0.00263	-0.02123	0.02820
	DS* (-4 < x_f, y_f, z_f < 5)	-0.00011	0.01838	-0.00263	-0.02120	0.02818
	DS* (-3 < x_f, y_f, z_f < 4)	-0.00005	0.01838	-0.00263	-0.02119	0.02817
	DS* (-2 < x_f, y_f, z_f < 3)	0.00010	0.01839	-0.00263	-0.02114	0.02814
	DS* (-1 < x_f, y_f, z_f < 2)	0.00062	0.01835	-0.00263	-0.02098	0.02799
H7	Single molecule	-1.11143	0.00802	0.00188	0.00139	0.00835
	ES*	0.04035	0.00475	-0.00988	-0.00432	0.01178
	DS* (-4 < x_f, y_f, z_f < 5)	0.05733	0.00475	-0.00988	-0.00433	0.01178
	DS* (-3 < x_f, y_f, z_f < 4)	0.05734	0.00475	-0.00988	-0.00433	0.01178
	DS* (-2 < x_f, y_f, z_f < 3)	0.05736	0.00474	-0.00988	-0.00433	0.01179
	DS* (-1 < x_f, y_f, z_f < 2)	0.05751	0.00473	-0.00988	-0.00435	0.01179
H8	Single molecule	-1.08336	0.01149	-0.00504	0.00381	0.01311
	ES*	0.01674	-0.00343	0.00207	-0.01170	0.01237
	DS* (-4 < x_f, y_f, z_f < 5)	0.03373	-0.00343	0.00206	-0.01169	0.01235
	DS* (-3 < x_f, y_f, z_f < 4)	0.03375	-0.00342	0.00205	-0.01168	0.01234
	DS* (-2 < x_f, y_f, z_f < 3)	0.03380	-0.00342	0.00204	-0.01166	0.01232
	DS* (-1 < x_f, y_f, z_f < 2)	0.03404	-0.00341	0.00201	-0.01159	0.01224
H9	Single molecule	-1.11327	0.00922	0.00630	0.00615	0.01274
	ES*	0.02235	0.00458	-0.00448	-0.00440	0.00776
	DS* (-4 < x_f, y_f, z_f < 5)	0.03932	0.00458	-0.00449	-0.00439	0.00777
	DS* (-3 < x_f, y_f, z_f < 4)	0.03932	0.00458	-0.00449	-0.00439	0.00778
	DS* (-2 < x_f, y_f, z_f < 3)	0.03933	0.00459	-0.00451	-0.00438	0.00779
	DS* (-1 < x_f, y_f, z_f < 2)	0.03942	0.00460	-0.00456	-0.00436	0.00781

Table S26 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **PARA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.024591	-1305.812773	-1306.600054	0.848291	-0.009062	0.994320
	ES*	-0.006708	0.001486	0.003044	0.000583	0.005180	-0.005277
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.006707	0.001490	0.003040	0.000582	0.005178	-0.005276
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.006706	0.001492	0.003037	0.000581	0.005177	-0.005274
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.006705	0.001497	0.003030	0.000578	0.005173	-0.005271
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006647	0.001536	0.002934	0.000564	0.005188	-0.005244
O2	Single molecule	-1305.771883	-1305.737011	-1305.853982	-0.600744	0.635175	-0.577483
	ES*	0.006057	0.003906	-0.014714	-0.002513	-0.001598	-0.005008
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.006058	0.003910	-0.014718	-0.002515	-0.001599	-0.005006
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.006058	0.003912	-0.014721	-0.002515	-0.001600	-0.005005
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.006060	0.003918	-0.014728	-0.002517	-0.001603	-0.005002
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.006065	0.003939	-0.014754	-0.002523	-0.001614	-0.004990
N1	Single molecule	-863.117029	-862.864623	-863.213438	0.265078	0.106905	0.195274
	ES*	0.001530	-0.001815	-0.000003	-0.000160	-0.002594	0.000236
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001531	-0.001812	-0.000008	-0.000162	-0.002595	0.000237
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001531	-0.001809	-0.000010	-0.000162	-0.002597	0.000239
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001532	-0.001803	-0.000017	-0.000164	-0.002599	0.000242
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001532	-0.001788	-0.000032	-0.000167	-0.002598	0.000260
C1	Single molecule	-534.469238	-534.604077	-534.502115	0.023771	-0.145657	-0.155096
	ES*	0.001357	-0.000338	-0.001161	-0.000388	-0.001252	0.000451
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001358	-0.000335	-0.001165	-0.000389	-0.001253	0.000453
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001358	-0.000332	-0.001168	-0.000390	-0.001255	0.000454
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001360	-0.000327	-0.001175	-0.000392	-0.001258	0.000457
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001354	-0.000311	-0.001184	-0.000391	-0.001264	0.000492
C2	Single molecule	-533.952630	-534.149724	-534.132772	-0.106260	-0.074113	-0.147514
	ES*	0.001726	-0.001430	-0.000380	0.000142	-0.002515	-0.000037
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001727	-0.001427	-0.000384	0.000141	-0.002516	-0.000035
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001727	-0.001424	-0.000387	0.000140	-0.002517	-0.000034
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001729	-0.001418	-0.000394	0.000138	-0.002520	-0.000031
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001729	-0.001401	-0.000412	0.000133	-0.002536	-0.000004
C3	Single molecule	-534.020255	-534.114206	-534.098946	-0.090761	-0.056007	-0.187126
	ES*	0.000282	-0.000452	0.000092	0.001172	-0.002419	-0.001441
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000283	-0.000449	0.000088	0.001170	-0.002421	-0.001439
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000283	-0.000446	0.000085	0.001170	-0.002422	-0.001438
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000285	-0.000440	0.000077	0.001167	-0.002425	-0.001435
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000297	-0.000417	0.000043	0.001156	-0.002442	-0.001403

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C4	Single molecule	-534.397992	-534.548039	-534.517021	-0.088028	-0.078720	-0.167586
	ES*	-0.001453	0.000780	0.000558	0.000165	-0.000013	-0.003119
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001452	0.000783	0.000553	0.000163	-0.000014	-0.003117
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001451	0.000786	0.000551	0.000163	-0.000016	-0.003115
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001450	0.000791	0.000543	0.000160	-0.000019	-0.003112
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001431	0.000837	0.000478	0.000146	-0.000033	-0.003056
C5	Single molecule	-533.961453	-534.148197	-534.123670	-0.095206	-0.079823	-0.148300
	ES*	0.000404	0.001554	-0.002075	-0.001029	0.000761	-0.001159
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000404	0.001557	-0.002079	-0.001030	0.000760	-0.001157
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000405	0.001560	-0.002082	-0.001031	0.000758	-0.001155
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000406	0.001565	-0.002089	-0.001034	0.000755	-0.001152
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000411	0.001643	-0.002172	-0.001030	0.000741	-0.001054
C6	Single molecule	-534.026445	-534.121838	-534.085607	-0.090931	-0.051170	-0.192059
	ES*	0.001286	0.001338	-0.002710	-0.000696	0.000041	-0.000321
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001287	0.001341	-0.002714	-0.000697	0.000040	-0.000319
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001287	0.001344	-0.002717	-0.000698	0.000039	-0.000318
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001288	0.001349	-0.002723	-0.000700	0.000036	-0.000314
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001283	0.001380	-0.002748	-0.000683	0.000032	-0.000240
C7	Single molecule	-534.592821	-534.805501	-534.456457	-0.152194	-0.137036	-0.127292
	ES*	0.000453	0.000037	-0.000668	-0.000439	0.000399	-0.000921
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000454	0.000041	-0.000672	-0.000440	0.000398	-0.000919
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000454	0.000044	-0.000675	-0.000441	0.000397	-0.000918
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000455	0.000049	-0.000682	-0.000443	0.000394	-0.000915
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000460	0.000069	-0.000706	-0.000450	0.000388	-0.000903
C8	Single molecule	-533.295558	-533.283548	-533.300272	0.006103	0.002875	0.006392
	ES*	-0.002372	0.000005	0.002132	0.000409	0.001696	-0.002725
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002371	0.000009	0.002128	0.000408	0.001695	-0.002723
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002371	0.000011	0.002125	0.000407	0.001694	-0.002722
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002370	0.000017	0.002118	0.000405	0.001691	-0.002719
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002362	0.000037	0.002089	0.000395	0.001686	-0.002708
H1	Single molecule	-1.920922	-2.078893	-2.175151	-0.056798	0.084326	0.235355
	ES*	0.004151	-0.003116	-0.002322	0.000239	-0.002355	0.001571
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004151	-0.003112	-0.002326	0.000238	-0.002356	0.001573
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004152	-0.003110	-0.002329	0.000237	-0.002357	0.001574
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004153	-0.003104	-0.002336	0.000235	-0.002360	0.001577
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004156	-0.003086	-0.002356	0.000230	-0.002375	0.001593
H2	Single molecule	-2.298737	-1.890405	-1.983356	-0.000194	0.195498	0.010058
	ES*	0.000663	-0.000304	-0.000885	0.000409	-0.002545	-0.001592
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000664	-0.000300	-0.000889	0.000408	-0.002546	-0.001590
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000664	-0.000297	-0.000892	0.000407	-0.002547	-0.001589
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000667	-0.000292	-0.000900	0.000405	-0.002550	-0.001586
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000686	-0.000272	-0.000939	0.000391	-0.002561	-0.001568

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H3	Single molecule	-1.923661	-2.063587	-2.176624	-0.048568	0.074632	0.230779
	ES*	0.002562	-0.000072	-0.003284	-0.001125	0.001991	0.002153
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002563	-0.000069	-0.003288	-0.001126	0.001989	0.002155
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002563	-0.000067	-0.003291	-0.001127	0.001988	0.002156
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002564	-0.000061	-0.003298	-0.001129	0.001985	0.002159
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002595	0.000122	-0.003512	-0.001117	0.001978	0.002266
H4	Single molecule	-2.285964	-1.897740	-1.983397	0.010776	0.186128	0.010489
	ES*	0.002041	0.002413	-0.004886	-0.004168	0.001026	-0.000072
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002042	0.002417	-0.004890	-0.004169	0.001025	-0.000070
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002042	0.002419	-0.004893	-0.004170	0.001023	-0.000068
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002043	0.002425	-0.004899	-0.004172	0.001021	-0.000065
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002049	0.002458	-0.004939	-0.004125	0.001024	0.000003
H5	Single molecule	-1.825928	-1.871904	-2.275950	-0.021912	0.092654	0.200901
	ES*	-0.009955	-0.008113	0.001811	-0.000381	0.003221	-0.004242
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.009955	-0.008109	0.001806	-0.000382	0.003219	-0.004240
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.009954	-0.008107	0.001804	-0.000383	0.003218	-0.004239
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.009953	-0.008102	0.001797	-0.000385	0.003214	-0.004235
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.009863	-0.008027	0.001632	-0.000391	0.003246	-0.004223
H6	Single molecule	-2.191871	-1.859236	-2.145289	0.061862	0.294217	-0.004805
	ES*	0.004876	-0.008372	-0.002275	0.001757	-0.009476	-0.002663
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004877	-0.008368	-0.002279	0.001755	-0.009477	-0.002661
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004877	-0.008365	-0.002282	0.001755	-0.009479	-0.002660
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004878	-0.008360	-0.002289	0.001753	-0.009481	-0.002657
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004883	-0.008344	-0.002309	0.001751	-0.009468	-0.002640
H7	Single molecule	-2.046546	-1.964312	-2.330386	-0.029283	-0.185371	-0.067553
	ES*	-0.002430	-0.000574	0.000994	0.000782	0.002200	-0.003815
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002430	-0.000570	0.000989	0.000781	0.002199	-0.003813
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002429	-0.000568	0.000987	0.000780	0.002198	-0.003812
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002429	-0.000562	0.000980	0.000778	0.002195	-0.003809
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002420	-0.000539	0.000948	0.000768	0.002188	-0.003800
H8	Single molecule	-2.166558	-1.970844	-2.213771	-0.058037	0.231247	0.078676
	ES*	-0.004245	-0.000347	0.004084	0.001709	0.001984	-0.004962
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.004244	-0.000343	0.004080	0.001707	0.001983	-0.004960
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.004244	-0.000341	0.004077	0.001707	0.001982	-0.004959
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.004243	-0.000335	0.004071	0.001705	0.001979	-0.004956
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.004234	-0.000313	0.004039	0.001693	0.001975	-0.004942
H9	Single molecule	-1.982997	-2.386349	-1.960190	-0.091375	-0.004810	-0.018299
	ES*	-0.003298	0.000587	0.001671	-0.001291	0.001351	-0.002035
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003297	0.000591	0.001667	-0.001292	0.001349	-0.002034
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003297	0.000594	0.001664	-0.001293	0.001348	-0.002032
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003296	0.000600	0.001657	-0.001295	0.001346	-0.002030
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003286	0.000616	0.001631	-0.001306	0.001339	-0.002020

Table S27 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **PARA** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	0.181822	0.499550	-0.681372	1.272436	-0.013593	1.491479
	ES*	-0.008973	0.003318	0.005655	0.000874	0.007770	-0.007916
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.008972	0.003323	0.005649	0.000872	0.007767	-0.007913
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.008971	0.003326	0.005645	0.000871	0.007765	-0.007911
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.008968	0.003334	0.005634	0.000868	0.007760	-0.007907
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.008882	0.003392	0.005490	0.000846	0.007782	-0.007867
O2	Single molecule	0.023613	0.075921	-0.099535	-0.901116	0.952762	-0.866225
	ES*	0.011461	0.008235	-0.019696	-0.003770	-0.002397	-0.007512
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.011462	0.008240	-0.019702	-0.003772	-0.002399	-0.007509
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.011463	0.008244	-0.019706	-0.003773	-0.002401	-0.007507
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.011464	0.008253	-0.019717	-0.003776	-0.002404	-0.007503
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.011472	0.008283	-0.019755	-0.003785	-0.002422	-0.007484
N1	Single molecule	-0.077998	0.300610	-0.222612	0.397618	0.160358	0.292912
	ES*	0.002439	-0.002579	0.000139	-0.000241	-0.003891	0.000353
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002440	-0.002573	0.000133	-0.000242	-0.003893	0.000356
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002441	-0.002570	0.000129	-0.000244	-0.003895	0.000358
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002442	-0.002561	0.000119	-0.000247	-0.003899	0.000362
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002442	-0.002538	0.000096	-0.000251	-0.003898	0.000390
C1	Single molecule	0.083858	-0.118400	0.034542	0.035656	-0.218486	-0.232644
	ES*	0.002107	-0.000437	-0.001671	-0.000581	-0.001878	0.000677
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002108	-0.000431	-0.001677	-0.000583	-0.001880	0.000680
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002109	-0.000428	-0.001681	-0.000584	-0.001882	0.000681
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002110	-0.000419	-0.001691	-0.000587	-0.001886	0.000686
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002101	-0.000396	-0.001706	-0.000586	-0.001896	0.000738
C2	Single molecule	0.188617	-0.107023	-0.081594	-0.159390	-0.111169	-0.221271
	ES*	0.002631	-0.002103	-0.000528	0.000214	-0.003772	-0.000055
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002632	-0.002098	-0.000534	0.000212	-0.003774	-0.000053
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002633	-0.002094	-0.000539	0.000210	-0.003776	-0.000051
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002635	-0.002085	-0.000550	0.000207	-0.003780	-0.000046
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002636	-0.002059	-0.000576	0.000199	-0.003804	-0.000006
C3	Single molecule	0.086321	-0.054606	-0.031715	-0.136142	-0.084011	-0.280689
	ES*	0.000462	-0.000639	0.000177	0.001757	-0.003629	-0.002161
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000463	-0.000634	0.000171	0.001756	-0.003631	-0.002159
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000464	-0.000630	0.000166	0.001754	-0.003633	-0.002157
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000467	-0.000622	0.000155	0.001751	-0.003638	-0.002153
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000484	-0.000587	0.000103	0.001734	-0.003663	-0.002104

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C4	Single molecule	0.134537	-0.090532	-0.044005	-0.132042	-0.118079	-0.251379
	ES*	-0.002121	0.001227	0.000894	0.000247	-0.000019	-0.004678
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.002120	0.001232	0.000888	0.000245	-0.000022	-0.004675
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.002120	0.001236	0.000884	0.000244	-0.000023	-0.004673
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.002117	0.001244	0.000873	0.000241	-0.000028	-0.004669
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.002088	0.001314	0.000775	0.000220	-0.000050	-0.004584
C5	Single molecule	0.174480	-0.105636	-0.068845	-0.142809	-0.119734	-0.222450
	ES*	0.000665	0.002390	-0.003054	-0.001544	0.001142	-0.001738
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000665	0.002395	-0.003060	-0.001546	0.001139	-0.001735
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000666	0.002398	-0.003064	-0.001547	0.001138	-0.001733
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000668	0.002407	-0.003075	-0.001550	0.001133	-0.001728
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000676	0.002523	-0.003199	-0.001544	0.001112	-0.001581
C6	Single molecule	0.077278	-0.065812	-0.011466	-0.136397	-0.076755	-0.288088
	ES*	0.001972	0.002049	-0.004022	-0.001043	0.000062	-0.000481
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001973	0.002055	-0.004028	-0.001045	0.000060	-0.000478
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001973	0.002058	-0.004032	-0.001047	0.000058	-0.000476
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001975	0.002067	-0.004042	-0.001050	0.000053	-0.000471
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001967	0.002113	-0.004080	-0.001024	0.000048	-0.000360
C7	Single molecule	0.038158	-0.280862	0.242704	-0.228291	-0.205554	-0.190938
	ES*	0.000769	0.000145	-0.000914	-0.000659	0.000599	-0.001382
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000770	0.000150	-0.000920	-0.000661	0.000596	-0.001379
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000770	0.000154	-0.000924	-0.000662	0.000595	-0.001377
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000772	0.000163	-0.000934	-0.000665	0.000591	-0.001373
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000778	0.000192	-0.000970	-0.000675	0.000582	-0.001355
C8	Single molecule	-0.003648	0.014367	-0.010719	0.009154	0.004312	0.009588
	ES*	-0.003440	0.000125	0.003315	0.000613	0.002544	-0.004087
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.003439	0.000130	0.003309	0.000611	0.002542	-0.004084
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.003439	0.000134	0.003305	0.000610	0.002541	-0.004083
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.003437	0.000143	0.003294	0.000607	0.002537	-0.004078
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.003425	0.000173	0.003252	0.000592	0.002528	-0.004063
H1	Single molecule	0.206100	-0.030856	-0.175244	-0.085197	0.126488	0.353033
	ES*	0.006870	-0.004030	-0.002839	0.000359	-0.003532	0.002356
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.006870	-0.004025	-0.002846	0.000357	-0.003534	0.002359
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.006871	-0.004021	-0.002850	0.000356	-0.003536	0.002361
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.006873	-0.004012	-0.002861	0.000353	-0.003540	0.002365
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.006877	-0.003986	-0.002891	0.000345	-0.003563	0.002389
H2	Single molecule	-0.361856	0.250641	0.111215	-0.000291	0.293246	0.015087
	ES*	0.001257	-0.000193	-0.001065	0.000614	-0.003817	-0.002388
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001258	-0.000187	-0.001071	0.000612	-0.003819	-0.002386
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001259	-0.000184	-0.001076	0.000610	-0.003821	-0.002384
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001262	-0.000175	-0.001087	0.000607	-0.003826	-0.002380
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001291	-0.000145	-0.001146	0.000586	-0.003842	-0.002352

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H3	Single molecule	0.196445	-0.013444	-0.183000	-0.072852	0.111948	0.346168
	ES*	0.004241	0.000289	-0.004529	-0.001687	0.002986	0.003229
	DS* (-4 < x_f, y_f, z_f < 5)	0.004241	0.000294	-0.004535	-0.001689	0.002984	0.003232
	DS* (-3 < x_f, y_f, z_f < 4)	0.004242	0.000297	-0.004539	-0.001690	0.002982	0.003234
	DS* (-2 < x_f, y_f, z_f < 3)	0.004243	0.000306	-0.004549	-0.001694	0.002978	0.003239
	DS* (-1 < x_f, y_f, z_f < 2)	0.004290	0.000580	-0.004870	-0.001676	0.002967	0.003399
H4	Single molecule	-0.345395	0.236940	0.108455	0.016163	0.279192	0.015734
	ES*	0.003278	0.003836	-0.007114	-0.006252	0.001539	-0.000107
	DS* (-4 < x_f, y_f, z_f < 5)	0.003279	0.003841	-0.007120	-0.006253	0.001537	-0.000105
	DS* (-3 < x_f, y_f, z_f < 4)	0.003279	0.003845	-0.007124	-0.006255	0.001535	-0.000103
	DS* (-2 < x_f, y_f, z_f < 3)	0.003280	0.003853	-0.007133	-0.006258	0.001531	-0.000097
	DS* (-1 < x_f, y_f, z_f < 2)	0.003289	0.003904	-0.007192	-0.006188	0.001535	0.000004
H5	Single molecule	0.247999	0.179034	-0.427033	-0.032868	0.138981	0.301351
	ES*	-0.006804	-0.004041	0.010845	-0.000572	0.004831	-0.006363
	DS* (-4 < x_f, y_f, z_f < 5)	-0.006803	-0.004035	0.010839	-0.000573	0.004828	-0.006360
	DS* (-3 < x_f, y_f, z_f < 4)	-0.006803	-0.004032	0.010834	-0.000575	0.004826	-0.006358
	DS* (-2 < x_f, y_f, z_f < 3)	-0.006800	-0.004025	0.010825	-0.000578	0.004821	-0.006353
	DS* (-1 < x_f, y_f, z_f < 2)	-0.006665	-0.003911	0.010576	-0.000586	0.004869	-0.006335
H6	Single molecule	-0.189609	0.309344	-0.119736	0.092792	0.441325	-0.007208
	ES*	0.010200	-0.009672	-0.000528	0.002635	-0.014214	-0.003995
	DS* (-4 < x_f, y_f, z_f < 5)	0.010201	-0.009667	-0.000534	0.002633	-0.014216	-0.003992
	DS* (-3 < x_f, y_f, z_f < 4)	0.010201	-0.009663	-0.000538	0.002632	-0.014218	-0.003990
	DS* (-2 < x_f, y_f, z_f < 3)	0.010202	-0.009654	-0.000548	0.002629	-0.014222	-0.003986
	DS* (-1 < x_f, y_f, z_f < 2)	0.010209	-0.009630	-0.000579	0.002627	-0.014203	-0.003959
H7	Single molecule	0.100802	0.224154	-0.324957	-0.043924	-0.278056	-0.101329
	ES*	-0.002640	0.000144	0.002496	0.001173	0.003300	-0.005722
	DS* (-4 < x_f, y_f, z_f < 5)	-0.002639	0.000150	0.002489	0.001171	0.003298	-0.005720
	DS* (-3 < x_f, y_f, z_f < 4)	-0.002639	0.000154	0.002485	0.001170	0.003297	-0.005718
	DS* (-2 < x_f, y_f, z_f < 3)	-0.002637	0.000162	0.002475	0.001167	0.003293	-0.005714
	DS* (-1 < x_f, y_f, z_f < 2)	-0.002625	0.000197	0.002427	0.001151	0.003282	-0.005700
H8	Single molecule	-0.074251	0.219320	-0.145070	-0.087056	0.346871	0.118014
	ES*	-0.006113	-0.000267	0.006380	0.002563	0.002976	-0.007442
	DS* (-4 < x_f, y_f, z_f < 5)	-0.006112	-0.000261	0.006374	0.002561	0.002974	-0.007440
	DS* (-3 < x_f, y_f, z_f < 4)	-0.006112	-0.000258	0.006370	0.002560	0.002972	-0.007438
	DS* (-2 < x_f, y_f, z_f < 3)	-0.006111	-0.000249	0.006360	0.002557	0.002968	-0.007434
	DS* (-1 < x_f, y_f, z_f < 2)	-0.006097	-0.000215	0.006312	0.002539	0.002963	-0.007413
H9	Single molecule	0.190273	-0.414756	0.224483	-0.137062	-0.007215	-0.027449
	ES*	-0.004427	0.001401	0.003026	-0.001937	0.002026	-0.003053
	DS* (-4 < x_f, y_f, z_f < 5)	-0.004426	0.001406	0.003020	-0.001939	0.002024	-0.003050
	DS* (-3 < x_f, y_f, z_f < 4)	-0.004426	0.001410	0.003016	-0.001940	0.002023	-0.003049
	DS* (-2 < x_f, y_f, z_f < 3)	-0.004425	0.001419	0.003006	-0.001943	0.002019	-0.003044
	DS* (-1 < x_f, y_f, z_f < 2)	-0.004409	0.001444	0.002966	-0.001959	0.002009	-0.003031

Table S28 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **SER** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.49745	0.23132	-0.18355	-0.10604	0.31375
	ES*	0.11188	-0.00199	0.01097	0.02936	0.03140
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.11249	-0.00200	0.01099	0.02931	0.03137
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.11239	-0.00201	0.01100	0.02928	0.03135
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.11216	-0.00202	0.01103	0.02921	0.03129
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.11126	-0.00150	0.01096	0.02889	0.03094
O2	Single molecule	-22.52412	-0.16660	0.08912	-0.25333	0.31603
	ES*	0.13979	0.00240	0.00143	0.02421	0.02437
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.14025	0.00240	0.00146	0.02413	0.02429
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.14004	0.00240	0.00148	0.02408	0.02424
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.13961	0.00241	0.00155	0.02397	0.02414
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.14071	0.00318	0.00227	0.02453	0.02484
O3	Single molecule	-22.38659	0.11433	0.03750	-0.33750	0.35831
	ES*	0.03477	0.00241	-0.00432	0.03420	0.03456
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.03539	0.00241	-0.00429	0.03414	0.03449
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.03529	0.00242	-0.00427	0.03410	0.03445
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.03504	0.00242	-0.00422	0.03399	0.03434
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.03355	0.00263	-0.00388	0.03339	0.03371
N1	Single molecule	-18.29986	-0.02877	0.01941	-0.04863	0.05974
	ES*	-0.04337	0.00511	-0.00198	0.02621	0.02678
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.04257	0.00513	-0.00198	0.02617	0.02675
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.04255	0.00515	-0.00198	0.02615	0.02673
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.04250	0.00519	-0.00198	0.02610	0.02668
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.04222	0.00540	-0.00197	0.02592	0.02655
C1	Single molecule	-14.80176	0.00799	-0.00283	-0.04776	0.04851
	ES*	0.09182	-0.00076	-0.00001	0.03014	0.03015
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.09242	-0.00076	0.00002	0.03007	0.03008
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.09231	-0.00076	0.00003	0.03003	0.03004
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.09206	-0.00075	0.00007	0.02994	0.02995
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.09212	-0.00016	0.00034	0.02995	0.02995
C2	Single molecule	-14.79195	-0.05041	0.02431	-0.05560	0.07889
	ES*	0.01393	0.00108	-0.00141	0.02810	0.02816
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01468	0.00111	-0.00139	0.02804	0.02810
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01467	0.00112	-0.00139	0.02800	0.02806
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01465	0.00117	-0.00136	0.02791	0.02797
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01503	0.00150	-0.00120	0.02772	0.02779

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C3	Single molecule	-14.79836	-0.07017	-0.00601	-0.00522	0.07062
	ES*	0.01605	0.00129	-0.00547	0.02444	0.02507
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.01677	0.00132	-0.00544	0.02436	0.02500
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.01674	0.00134	-0.00543	0.02432	0.02495
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.01666	0.00138	-0.00539	0.02420	0.02484
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.01651	0.00172	-0.00513	0.02380	0.02441
H1	Single molecule	-1.07840	0.00451	0.00460	-0.03373	0.03434
	ES*	-0.00138	-0.00086	0.00132	0.02355	0.02360
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.00052	-0.00082	0.00132	0.02348	0.02353
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.00046	-0.00079	0.00133	0.02344	0.02349
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.00030	-0.00072	0.00135	0.02334	0.02339
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.00089	-0.00039	0.00143	0.02320	0.02325
H2	Single molecule	-1.07812	-0.00923	0.01706	-0.02658	0.03291
	ES*	-0.02152	0.00945	-0.01192	0.01931	0.02458
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.02066	0.00949	-0.01190	0.01924	0.02453
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.02059	0.00952	-0.01189	0.01920	0.02450
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.02044	0.00959	-0.01187	0.01909	0.02443
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.01975	0.00992	-0.01172	0.01869	0.02419
H3	Single molecule	-1.14658	0.00717	-0.00179	-0.01109	0.01333
	ES*	0.04603	-0.00354	-0.00300	0.01907	0.01962
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.04667	-0.00351	-0.00297	0.01898	0.01953
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.04658	-0.00349	-0.00295	0.01892	0.01946
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.04636	-0.00345	-0.00290	0.01878	0.01931
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04594	-0.00306	-0.00255	0.01836	0.01879
H4	Single molecule	-0.91442	-0.02157	0.01314	-0.03704	0.04483
	ES*	-0.05706	0.01830	0.00143	0.02616	0.03196
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.05629	0.01831	0.00143	0.02613	0.03194
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.05630	0.01831	0.00143	0.02612	0.03193
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.05630	0.01833	0.00144	0.02608	0.03191
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.05633	0.01840	0.00148	0.02588	0.03179
H5	Single molecule	-0.88520	0.01300	0.01251	-0.02191	0.02838
	ES*	-0.08890	-0.00537	0.00260	0.02494	0.02564
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.08803	-0.00533	0.00259	0.02491	0.02560
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.08796	-0.00530	0.00258	0.02489	0.02558
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.08778	-0.00524	0.00257	0.02484	0.02552
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.08703	-0.00499	0.00251	0.02468	0.02530
H6	Single molecule	-0.91959	-0.00975	0.01343	-0.03177	0.03584
	ES*	-0.05237	0.00893	-0.01505	0.02710	0.03226
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.05159	0.00895	-0.01506	0.02708	0.03225
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.05158	0.00897	-0.01506	0.02706	0.03224
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.05155	0.00900	-0.01507	0.02702	0.03222
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.05140	0.00921	-0.01514	0.02690	0.03221

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H7	Single molecule	-0.97336	0.00688	0.01395	-0.03120	0.03486
	ES*	-0.01845	0.00141	-0.00385	0.03452	0.03476
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.01776	0.00142	-0.00383	0.03447	0.03471
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.01781	0.00143	-0.00381	0.03443	0.03467
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.01795	0.00144	-0.00377	0.03435	0.03458
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.01882	0.00155	-0.00354	0.03384	0.03406

Table S29 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **SER** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1306.299608	-1306.307684	-1304.809193	0.127184	0.382831	-0.089153
	ES*	0.004370	-0.011475	0.004792	0.006298	-0.002203	-0.000098
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004362	-0.011472	0.004796	0.006298	-0.002196	-0.000102
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004358	-0.011470	0.004799	0.006297	-0.002192	-0.000105
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004344	-0.011462	0.004805	0.006296	-0.002186	-0.000112
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004117	-0.011278	0.004848	0.006244	-0.002377	-0.000037
O2	Single molecule	-1305.867892	-1305.857388	-1305.681540	-0.348254	-0.673489	0.577726
	ES*	-0.014332	0.007691	0.003096	0.007210	0.009654	-0.004696
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.014339	0.007694	0.003100	0.007210	0.009660	-0.004701
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.014343	0.007697	0.003102	0.007209	0.009665	-0.004704
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.014348	0.007705	0.003098	0.007208	0.009670	-0.004714
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.014165	0.007881	0.002739	0.007140	0.009480	-0.004944
O3	Single molecule	-1306.962212	-1305.317915	-1306.463228	-0.990630	-0.273927	-0.253874
	ES*	0.001737	0.001587	-0.004428	-0.000156	0.002178	0.001121
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001729	0.001591	-0.004424	-0.000156	0.002185	0.001116
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001725	0.001593	-0.004421	-0.000157	0.002189	0.001113
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001712	0.001598	-0.004414	-0.000157	0.002199	0.001105
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001604	0.001604	-0.004312	-0.000150	0.002166	0.001016
N1	Single molecule	-863.284412	-863.296028	-863.270610	-0.018822	0.042229	-0.017101
	ES*	0.001970	0.001253	-0.003569	-0.000575	-0.001396	0.000656
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001962	0.001257	-0.003565	-0.000575	-0.001389	0.000651
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001957	0.001259	-0.003562	-0.000575	-0.001385	0.000648
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001945	0.001265	-0.003556	-0.000575	-0.001375	0.000639
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001883	0.001311	-0.003539	-0.000579	-0.001379	0.000598
C1	Single molecule	-534.015596	-534.202335	-533.967106	-0.274701	0.091926	0.018970
	ES*	0.000302	0.000732	-0.001452	0.002296	0.000836	-0.000618
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000295	0.000736	-0.001448	0.002296	0.000843	-0.000622
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000291	0.000738	-0.001445	0.002296	0.000847	-0.000625
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000280	0.000745	-0.001442	0.002295	0.000854	-0.000634
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000252	0.000893	-0.001563	0.002251	0.000683	-0.000703
C2	Single molecule	-534.063989	-533.916973	-534.036400	0.113238	-0.171598	0.101339
	ES*	0.001511	-0.000808	-0.000750	-0.000469	0.000852	-0.000114
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001504	-0.000804	-0.000746	-0.000469	0.000859	-0.000119
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001499	-0.000802	-0.000744	-0.000469	0.000864	-0.000122
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001488	-0.000796	-0.000738	-0.000470	0.000874	-0.000130
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001462	-0.000739	-0.000769	-0.000473	0.000838	-0.000197

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C3	Single molecule	-534.019257	-533.825496	-533.753611	-0.104353	0.072157	0.022449
	ES*	0.002364	-0.001426	-0.001079	0.001345	0.003137	-0.002153
	DS* (-4 < x_f, y_f, z_f < 5)	0.002357	-0.001422	-0.001075	0.001345	0.003144	-0.002158
	DS* (-3 < x_f, y_f, z_f < 4)	0.002352	-0.001420	-0.001072	0.001345	0.003149	-0.002161
	DS* (-2 < x_f, y_f, z_f < 3)	0.002341	-0.001414	-0.001066	0.001345	0.003159	-0.002170
	DS* (-1 < x_f, y_f, z_f < 2)	0.002308	-0.001393	-0.001054	0.001351	0.003133	-0.002242
H1	Single molecule	-2.243480	-1.982223	-1.954387	-0.136019	0.087131	0.048724
	ES*	0.002229	-0.000056	-0.002638	-0.001374	0.003144	0.001944
	DS* (-4 < x_f, y_f, z_f < 5)	0.002221	-0.000052	-0.002634	-0.001374	0.003151	0.001939
	DS* (-3 < x_f, y_f, z_f < 4)	0.002216	-0.000050	-0.002632	-0.001374	0.003156	0.001936
	DS* (-2 < x_f, y_f, z_f < 3)	0.002206	-0.000044	-0.002627	-0.001374	0.003168	0.001927
	DS* (-1 < x_f, y_f, z_f < 2)	0.002216	0.000003	-0.002684	-0.001368	0.003172	0.001866
H2	Single molecule	-1.965337	-1.957477	-2.313785	0.013268	0.084990	-0.091447
	ES*	0.003060	-0.001536	-0.002185	0.004635	0.004466	-0.002174
	DS* (-4 < x_f, y_f, z_f < 5)	0.003053	-0.001532	-0.002181	0.004635	0.004473	-0.002178
	DS* (-3 < x_f, y_f, z_f < 4)	0.003047	-0.001530	-0.002178	0.004635	0.004478	-0.002181
	DS* (-2 < x_f, y_f, z_f < 3)	0.003035	-0.001524	-0.002172	0.004635	0.004489	-0.002189
	DS* (-1 < x_f, y_f, z_f < 2)	0.002991	-0.001498	-0.002154	0.004638	0.004493	-0.002239
H3	Single molecule	-2.140532	-2.002071	-2.094523	0.110973	-0.181853	0.113552
	ES*	0.001561	-0.001275	-0.000943	0.002511	0.000933	-0.008194
	DS* (-4 < x_f, y_f, z_f < 5)	0.001554	-0.001271	-0.000939	0.002511	0.000939	-0.008199
	DS* (-3 < x_f, y_f, z_f < 4)	0.001549	-0.001269	-0.000936	0.002510	0.000944	-0.008202
	DS* (-2 < x_f, y_f, z_f < 3)	0.001540	-0.001264	-0.000932	0.002510	0.000955	-0.008210
	DS* (-1 < x_f, y_f, z_f < 2)	0.001575	-0.001274	-0.000957	0.002521	0.000923	-0.008287
H4	Single molecule	-2.174772	-1.831964	-1.759270	-0.169927	0.050979	0.019919
	ES*	0.011192	-0.005144	-0.013102	0.004052	0.000854	0.000335
	DS* (-4 < x_f, y_f, z_f < 5)	0.011184	-0.005140	-0.013098	0.004052	0.000860	0.000331
	DS* (-3 < x_f, y_f, z_f < 4)	0.011179	-0.005138	-0.013095	0.004052	0.000865	0.000328
	DS* (-2 < x_f, y_f, z_f < 3)	0.011167	-0.005132	-0.013089	0.004051	0.000875	0.000320
	DS* (-1 < x_f, y_f, z_f < 2)	0.011086	-0.005083	-0.013057	0.004049	0.000897	0.000276
H5	Single molecule	-1.811276	-1.771432	-2.187309	0.021044	0.142361	-0.057195
	ES*	0.002907	-0.005248	-0.005774	-0.006177	-0.007954	0.002169
	DS* (-4 < x_f, y_f, z_f < 5)	0.002900	-0.005244	-0.005770	-0.006178	-0.007948	0.002165
	DS* (-3 < x_f, y_f, z_f < 4)	0.002895	-0.005242	-0.005768	-0.006178	-0.007943	0.002162
	DS* (-2 < x_f, y_f, z_f < 3)	0.002882	-0.005236	-0.005761	-0.006178	-0.007933	0.002153
	DS* (-1 < x_f, y_f, z_f < 2)	0.002834	-0.005200	-0.005749	-0.006177	-0.007929	0.002106
H6	Single molecule	-1.774031	-2.237985	-1.765267	0.047704	0.004346	-0.060833
	ES*	-0.006825	0.011050	-0.011956	-0.004459	0.001349	-0.001162
	DS* (-4 < x_f, y_f, z_f < 5)	-0.006833	0.011054	-0.011951	-0.004459	0.001356	-0.001166
	DS* (-3 < x_f, y_f, z_f < 4)	-0.006838	0.011056	-0.011949	-0.004460	0.001360	-0.001169
	DS* (-2 < x_f, y_f, z_f < 3)	-0.006850	0.011061	-0.011942	-0.004460	0.001370	-0.001178
	DS* (-1 < x_f, y_f, z_f < 2)	-0.006918	0.011098	-0.011911	-0.004467	0.001359	-0.001200

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-1.953008	-1.847591	-2.297095	-0.099734	-0.255414	-0.157488
	ES*	-0.005821	-0.001502	0.003834	-0.000715	-0.003307	-0.000081
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.005829	-0.001498	0.003838	-0.000715	-0.003300	-0.000086
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.005834	-0.001496	0.003841	-0.000715	-0.003296	-0.000089
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.005847	-0.001490	0.003848	-0.000716	-0.003285	-0.000096
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.005936	-0.001481	0.003927	-0.000715	-0.003275	-0.000156

Table S30 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **SER** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-0.741169	-0.753284	1.494453	0.190775	0.574246	-0.133730
	ES*	0.007711	-0.016056	0.008345	0.009447	-0.003304	-0.000147
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.007700	-0.016051	0.008351	0.009446	-0.003294	-0.000154
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.007693	-0.016048	0.008354	0.009446	-0.003288	-0.000158
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.007673	-0.016037	0.008364	0.009444	-0.003278	-0.000168
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.007332	-0.015761	0.008429	0.009365	-0.003565	-0.000056
O2	Single molecule	-0.098428	-0.082672	0.181100	-0.522381	-1.010233	0.866589
	ES*	-0.019725	0.013309	0.006416	0.010815	0.014480	-0.007044
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.019736	0.013314	0.006422	0.010814	0.014491	-0.007051
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.019743	0.013317	0.006425	0.010814	0.014498	-0.007056
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.019750	0.013330	0.006420	0.010812	0.014505	-0.007072
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.019475	0.013594	0.005882	0.010710	0.014220	-0.007416
O3	Single molecule	-1.071640	1.394804	-0.323164	-1.485945	-0.410891	-0.380811
	ES*	0.003157	0.002932	-0.006090	-0.000234	0.003267	0.001681
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003146	0.002938	-0.006084	-0.000235	0.003277	0.001674
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003139	0.002941	-0.006080	-0.000235	0.003284	0.001670
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003120	0.002949	-0.006069	-0.000236	0.003299	0.001657
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002958	0.002958	-0.005916	-0.000225	0.003249	0.001523
N1	Single molecule	-0.001093	-0.018517	0.019610	-0.028233	0.063343	-0.025651
	ES*	0.003128	0.002053	-0.005181	-0.000862	-0.002094	0.000983
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003116	0.002058	-0.005175	-0.000862	-0.002084	0.000976
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003109	0.002062	-0.005171	-0.000862	-0.002078	0.000972
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003090	0.002071	-0.005161	-0.000863	-0.002063	0.000959
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002997	0.002139	-0.005136	-0.000868	-0.002069	0.000897
C1	Single molecule	0.069125	-0.210984	0.141859	-0.412052	0.137889	0.028455
	ES*	0.000662	0.001307	-0.001969	0.003444	0.001254	-0.000927
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000651	0.001312	-0.001963	0.003444	0.001264	-0.000933
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000644	0.001315	-0.001960	0.003444	0.001271	-0.000938
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000629	0.001326	-0.001955	0.003442	0.001282	-0.000951
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000587	0.001549	-0.002136	0.003376	0.001025	-0.001055
C2	Single molecule	-0.087302	0.133221	-0.045919	0.169856	-0.257397	0.152009
	ES*	0.002290	-0.001188	-0.001102	-0.000703	0.001278	-0.000171
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002279	-0.001183	-0.001096	-0.000703	0.001289	-0.000178
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002272	-0.001180	-0.001092	-0.000703	0.001295	-0.000183
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002255	-0.001171	-0.001084	-0.000704	0.001311	-0.000196
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002216	-0.001085	-0.001131	-0.000710	0.001258	-0.000295

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C3	Single molecule	-0.229704	0.060939	0.168766	-0.156530	0.108236	0.033674
	ES*	0.003616	-0.002068	-0.001548	0.002018	0.004706	-0.003230
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003605	-0.002063	-0.001542	0.002018	0.004716	-0.003237
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003598	-0.002059	-0.001538	0.002018	0.004723	-0.003242
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003581	-0.002051	-0.001529	0.002017	0.004739	-0.003254
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003532	-0.002020	-0.001512	0.002026	0.004699	-0.003363
H1	Single molecule	-0.275175	0.116711	0.158464	-0.204028	0.130697	0.073085
	ES*	0.003576	0.000149	-0.003725	-0.002060	0.004717	0.002916
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.003564	0.000154	-0.003719	-0.002061	0.004727	0.002909
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.003557	0.000158	-0.003715	-0.002061	0.004734	0.002904
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.003541	0.000166	-0.003707	-0.002062	0.004752	0.002891
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.003556	0.000238	-0.003794	-0.002052	0.004758	0.002800
H2	Single molecule	0.170294	0.182084	-0.352378	0.019901	0.127485	-0.137171
	ES*	0.004921	-0.001973	-0.002947	0.006953	0.006699	-0.003261
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004909	-0.001968	-0.002941	0.006953	0.006710	-0.003267
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004902	-0.001964	-0.002937	0.006953	0.006717	-0.003272
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004883	-0.001956	-0.002927	0.006952	0.006733	-0.003284
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004817	-0.001916	-0.002901	0.006957	0.006740	-0.003358
H3	Single molecule	-0.092235	0.115457	-0.023222	0.166459	-0.272780	0.170328
	ES*	0.002670	-0.001584	-0.001086	0.003766	0.001399	-0.012291
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.002659	-0.001578	-0.001080	0.003766	0.001409	-0.012298
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.002651	-0.001575	-0.001077	0.003766	0.001416	-0.012303
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.002638	-0.001568	-0.001070	0.003765	0.001433	-0.012316
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.002690	-0.001582	-0.001108	0.003782	0.001384	-0.012430
H4	Single molecule	-0.379155	0.135057	0.244098	-0.254891	0.076468	0.029879
	ES*	0.020315	-0.004189	-0.016126	0.006078	0.001281	0.000503
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.020303	-0.004184	-0.016120	0.006078	0.001291	0.000496
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.020296	-0.004180	-0.016116	0.006078	0.001297	0.000491
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.020277	-0.004171	-0.016106	0.006077	0.001312	0.000479
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.020156	-0.004097	-0.016059	0.006074	0.001345	0.000414
H5	Single molecule	0.168094	0.227861	-0.395955	0.031566	0.213541	-0.085793
	ES*	0.008419	-0.003814	-0.004604	-0.009266	-0.011931	0.003254
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.008407	-0.003809	-0.004598	-0.009266	-0.011921	0.003247
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.008399	-0.003805	-0.004594	-0.009267	-0.011915	0.003242
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.008380	-0.003796	-0.004584	-0.009267	-0.011899	0.003230
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.008308	-0.003742	-0.004566	-0.009265	-0.011893	0.003160
H6	Single molecule	0.227595	-0.468336	0.240741	0.071557	0.006519	-0.091250
	ES*	-0.006372	0.020440	-0.014068	-0.006689	0.002023	-0.001742
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.006384	0.020446	-0.014062	-0.006689	0.002033	-0.001749
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.006391	0.020449	-0.014058	-0.006689	0.002040	-0.001754
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.006410	0.020457	-0.014048	-0.006690	0.002054	-0.001766
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.006512	0.020513	-0.014001	-0.006701	0.002038	-0.001800

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	0.119335	0.277460	-0.396795	-0.149601	-0.383122	-0.236232
	ES*	-0.006988	-0.000508	0.007496	-0.001072	-0.004960	-0.000121
	DS* (-4 < x_f, y_f, z_f < 5)	-0.006999	-0.000503	0.007502	-0.001073	-0.004950	-0.000128
	DS* (-3 < x_f, y_f, z_f < 4)	-0.007007	-0.000499	0.007506	-0.001073	-0.004943	-0.000133
	DS* (-2 < x_f, y_f, z_f < 3)	-0.007025	-0.000491	0.007517	-0.001073	-0.004928	-0.000145
	DS* (-1 < x_f, y_f, z_f < 2)	-0.007159	-0.000477	0.007636	-0.001072	-0.004913	-0.000234

Table S31 Electrostatic potential (ESP) and electric field (EF) (all in atomic units) at the locations of the nuclei of the central **VAL** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
O1	Single molecule	-22.50432	0.16153	0.24869	0.07506	0.30590
	ES*	0.10731	0.01834	-0.03514	-0.00412	0.03985
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.05159	0.01836	-0.03510	-0.00412	0.03983
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.05150	0.01837	-0.03507	-0.00412	0.03981
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.05125	0.01839	-0.03497	-0.00414	0.03973
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.04942	0.01831	-0.03416	-0.00419	0.03898
O2	Single molecule	-22.52942	-0.29559	0.08870	-0.02437	0.30957
	ES*	0.13088	0.01818	-0.00713	-0.01249	0.02318
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.07523	0.01818	-0.00713	-0.01250	0.02319
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.07518	0.01818	-0.00714	-0.01251	0.02320
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.07503	0.01818	-0.00712	-0.01253	0.02320
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.07339	0.01792	-0.00663	-0.01263	0.02291
N1	Single molecule	-18.32553	-0.04718	0.01932	-0.02147	0.05532
	ES*	-0.03331	0.01541	-0.01576	0.00581	0.02279
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.08877	0.01536	-0.01570	0.00584	0.02273
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.08868	0.01533	-0.01566	0.00586	0.02269
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.08841	0.01526	-0.01554	0.00594	0.02258
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.08663	0.01485	-0.01477	0.00701	0.02209
H1	Single molecule	-0.93670	-0.03375	0.01651	0.00622	0.03808
	ES*	-0.04324	0.02362	-0.00376	0.00034	0.02392
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.09870	0.02358	-0.00368	0.00036	0.02387
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.09862	0.02356	-0.00363	0.00038	0.02384
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.09833	0.02349	-0.00347	0.00046	0.02375
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.09615	0.02297	-0.00255	0.00144	0.02316
H2	Single molecule	-0.91017	-0.01447	0.02511	-0.00514	0.02943
	ES*	-0.07998	0.01603	-0.02981	0.00186	0.03390
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.13529	0.01596	-0.02975	0.00190	0.03381
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.13510	0.01592	-0.02970	0.00193	0.03375
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.13451	0.01580	-0.02956	0.00207	0.03358
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.13055	0.01522	-0.02848	0.00378	0.03251
H3	Single molecule	-0.93920	-0.00036	0.01065	-0.02092	0.02348
	ES*	-0.04191	0.00838	-0.01382	0.01658	0.02315
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.09745	0.00835	-0.01377	0.01660	0.02313
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.09742	0.00833	-0.01374	0.01662	0.02312
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.09736	0.00828	-0.01367	0.01670	0.02311
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.09779	0.00817	-0.01342	0.01763	0.02362

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
C1	Single molecule	-14.80726	-0.02306	0.04178	0.00467	0.04795
	ES*	0.08541	0.01654	-0.02168	-0.00059	0.02727
	DS* (-4 < x_f, y_f, z_f < 5)	0.02976	0.01654	-0.02165	-0.00059	0.02725
	DS* (-3 < x_f, y_f, z_f < 4)	0.02972	0.01654	-0.02164	-0.00059	0.02724
	DS* (-2 < x_f, y_f, z_f < 3)	0.02960	0.01653	-0.02158	-0.00059	0.02718
	DS* (-1 < x_f, y_f, z_f < 2)	0.02871	0.01630	-0.02095	-0.00049	0.02655
C2	Single molecule	-14.81706	-0.07056	0.00619	-0.03252	0.07794
	ES*	0.01986	0.01647	-0.01641	0.00501	0.02378
	DS* (-4 < x_f, y_f, z_f < 5)	-0.03569	0.01643	-0.01638	0.00503	0.02373
	DS* (-3 < x_f, y_f, z_f < 4)	-0.03566	0.01640	-0.01635	0.00504	0.02370
	DS* (-2 < x_f, y_f, z_f < 3)	-0.03552	0.01632	-0.01626	0.00509	0.02360
	DS* (-1 < x_f, y_f, z_f < 2)	-0.03402	0.01584	-0.01541	0.00570	0.02282
H4	Single molecule	-1.11089	-0.00003	0.01880	-0.01554	0.02439
	ES*	0.01812	0.01732	-0.01535	0.00260	0.02329
	DS* (-4 < x_f, y_f, z_f < 5)	-0.03748	0.01727	-0.01534	0.00262	0.02325
	DS* (-3 < x_f, y_f, z_f < 4)	-0.03749	0.01723	-0.01534	0.00263	0.02322
	DS* (-2 < x_f, y_f, z_f < 3)	-0.03742	0.01713	-0.01528	0.00270	0.02311
	DS* (-1 < x_f, y_f, z_f < 2)	-0.03619	0.01654	-0.01459	0.00364	0.02236
C3	Single molecule	-14.82752	-0.01166	0.01670	0.00602	0.02124
	ES*	0.02260	0.01049	-0.01150	0.00655	0.01688
	DS* (-4 < x_f, y_f, z_f < 5)	-0.03286	0.01043	-0.01144	0.00657	0.01682
	DS* (-3 < x_f, y_f, z_f < 4)	-0.03276	0.01039	-0.01141	0.00659	0.01678
	DS* (-2 < x_f, y_f, z_f < 3)	-0.03241	0.01028	-0.01128	0.00662	0.01663
	DS* (-1 < x_f, y_f, z_f < 2)	-0.02894	0.00968	-0.01001	0.00673	0.01546
H5	Single molecule	-1.07208	-0.01311	0.00669	-0.01250	0.01931
	ES*	-0.00457	0.00677	-0.00969	0.01383	0.01819
	DS* (-4 < x_f, y_f, z_f < 5)	-0.05983	0.00669	-0.00962	0.01386	0.01815
	DS* (-3 < x_f, y_f, z_f < 4)	-0.05960	0.00664	-0.00957	0.01388	0.01812
	DS* (-2 < x_f, y_f, z_f < 3)	-0.05884	0.00649	-0.00939	0.01392	0.01800
	DS* (-1 < x_f, y_f, z_f < 2)	-0.05201	0.00580	-0.00748	0.01388	0.01680
C4	Single molecule	-14.88025	-0.02826	0.00581	-0.00429	0.02917
	ES*	0.04320	0.00885	-0.00986	0.00307	0.01360
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01237	0.00878	-0.00983	0.00309	0.01354
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01234	0.00873	-0.00982	0.00310	0.01350
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01216	0.00861	-0.00973	0.00311	0.01336
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00924	0.00795	-0.00856	0.00295	0.01205
H6	Single molecule	-1.13292	-0.01962	-0.00454	0.00066	0.02015
	ES*	0.02623	0.01025	-0.01325	0.00831	0.01870
	DS* (-4 < x_f, y_f, z_f < 5)	-0.02939	0.01017	-0.01324	0.00834	0.01866
	DS* (-3 < x_f, y_f, z_f < 4)	-0.02939	0.01011	-0.01323	0.00835	0.01863
	DS* (-2 < x_f, y_f, z_f < 3)	-0.02918	0.00995	-0.01313	0.00838	0.01848
	DS* (-1 < x_f, y_f, z_f < 2)	-0.02452	0.00896	-0.01138	0.00849	0.01679

ATOM	CALCULATION	ESP	EF(X)	EF(Y)	EF(Z)	|EF|
H7	Single molecule	-1.16807	-0.02035	0.01762	0.00593	0.02756
	ES*	0.07009	0.00933	-0.00927	-0.00477	0.01399
	DS* (-4 < x_f, y_f, z_f < 5)	0.01442	0.00928	-0.00926	-0.00477	0.01395
	DS* (-3 < x_f, y_f, z_f < 4)	0.01438	0.00925	-0.00926	-0.00477	0.01393
	DS* (-2 < x_f, y_f, z_f < 3)	0.01431	0.00916	-0.00921	-0.00476	0.01383
	DS* (-1 < x_f, y_f, z_f < 2)	0.01505	0.00863	-0.00846	-0.00465	0.01295
H8	Single molecule	-1.13310	-0.01256	-0.00060	-0.01565	0.02008
	ES*	0.04457	0.00436	-0.00446	0.00395	0.00738
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01092	0.00427	-0.00442	0.00397	0.00732
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01084	0.00422	-0.00439	0.00398	0.00728
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01058	0.00408	-0.00431	0.00397	0.00714
	DS* (-1 < x_f, y_f, z_f < 2)	-0.00783	0.00352	-0.00346	0.00320	0.00588
C5	Single molecule	-14.87850	-0.00337	0.03013	-0.00433	0.03062
	ES*	0.04088	0.00864	-0.00829	0.00396	0.01261
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01465	0.00860	-0.00821	0.00397	0.01254
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01460	0.00858	-0.00816	0.00398	0.01249
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01443	0.00851	-0.00801	0.00399	0.01235
	DS* (-1 < x_f, y_f, z_f < 2)	-0.01273	0.00802	-0.00711	0.00395	0.01142
H9	Single molecule	-1.12838	0.00098	0.02585	-0.00412	0.02619
	ES*	0.02332	0.01226	-0.00856	0.01043	0.01823
	DS* (-4 < x_f, y_f, z_f < 5)	-0.03223	0.01224	-0.00846	0.01044	0.01817
	DS* (-3 < x_f, y_f, z_f < 4)	-0.03219	0.01222	-0.00840	0.01045	0.01814
	DS* (-2 < x_f, y_f, z_f < 3)	-0.03202	0.01214	-0.00822	0.01048	0.01802
	DS* (-1 < x_f, y_f, z_f < 2)	-0.03000	0.01148	-0.00724	0.01054	0.01719
H10	Single molecule	-1.12951	0.00128	0.01133	-0.01790	0.02123
	ES*	0.04118	0.00483	-0.00498	0.00298	0.00755
	DS* (-4 < x_f, y_f, z_f < 5)	-0.01425	0.00478	-0.00489	0.00300	0.00747
	DS* (-3 < x_f, y_f, z_f < 4)	-0.01414	0.00475	-0.00483	0.00301	0.00741
	DS* (-2 < x_f, y_f, z_f < 3)	-0.01383	0.00466	-0.00467	0.00302	0.00725
	DS* (-1 < x_f, y_f, z_f < 2)	-0.01185	0.00425	-0.00396	0.00266	0.00639
H11	Single molecule	-1.16766	-0.01198	0.02427	0.00477	0.02748
	ES*	0.06602	0.00849	-0.00951	-0.00154	0.01284
	DS* (-4 < x_f, y_f, z_f < 5)	0.01035	0.00847	-0.00945	-0.00154	0.01279
	DS* (-3 < x_f, y_f, z_f < 4)	0.01030	0.00846	-0.00941	-0.00154	0.01275
	DS* (-2 < x_f, y_f, z_f < 3)	0.01020	0.00843	-0.00928	-0.00154	0.01263
	DS* (-1 < x_f, y_f, z_f < 2)	0.01010	0.00809	-0.00848	-0.00138	0.01180

Table S32 Elements of the unabridged electric field gradient (EFG) tensors $\nabla\mathbb{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **VAL** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	-1305.552080	-1305.773512	-1306.295447	-0.865040	-0.083250	-0.016131
	ES*	0.002133	-0.012232	0.006117	0.006004	-0.002446	-0.001926
	DS* (-4 < x_f, y_f, z_f < 5)	0.002131	-0.012231	0.006117	0.006018	-0.002442	-0.001931
	DS* (-3 < x_f, y_f, z_f < 4)	0.002130	-0.012229	0.006116	0.006027	-0.002440	-0.001935
	DS* (-2 < x_f, y_f, z_f < 3)	0.002126	-0.012220	0.006111	0.006048	-0.002428	-0.001952
	DS* (-1 < x_f, y_f, z_f < 2)	0.002082	-0.012069	0.006004	0.006112	-0.002299	-0.002133
O2	Single molecule	-1306.505898	-1304.911448	-1306.204704	0.285351	0.028542	0.335145
	ES*	-0.001102	-0.001792	-0.000594	-0.011702	0.007047	-0.004715
	DS* (-4 < x_f, y_f, z_f < 5)	-0.001103	-0.001790	-0.000594	-0.011688	0.007050	-0.004721
	DS* (-3 < x_f, y_f, z_f < 4)	-0.001104	-0.001789	-0.000594	-0.011680	0.007053	-0.004724
	DS* (-2 < x_f, y_f, z_f < 3)	-0.001104	-0.001783	-0.000601	-0.011657	0.007060	-0.004739
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001058	-0.001702	-0.000727	-0.011562	0.007129	-0.004886
N1	Single molecule	-863.342223	-863.407910	-863.393529	-0.008587	0.050098	-0.005052
	ES*	-0.000977	0.000212	0.000321	0.000601	-0.000943	0.000217
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000978	0.000213	0.000321	0.000614	-0.000940	0.000212
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000979	0.000214	0.000321	0.000623	-0.000938	0.000208
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000981	0.000211	0.000326	0.000643	-0.000926	0.000188
	DS* (-1 < x_f, y_f, z_f < 2)	-0.001004	0.000139	0.000421	0.000723	-0.000798	-0.000064
H1	Single molecule	-2.024086	-1.944708	-1.852155	-0.207474	0.127172	0.108775
	ES*	0.000637	-0.000624	-0.007407	0.012898	-0.002414	-0.007975
	DS* (-4 < x_f, y_f, z_f < 5)	0.000636	-0.000623	-0.007407	0.012911	-0.002411	-0.007981
	DS* (-3 < x_f, y_f, z_f < 4)	0.000634	-0.000622	-0.007407	0.012919	-0.002408	-0.007984
	DS* (-2 < x_f, y_f, z_f < 3)	0.000628	-0.000623	-0.007400	0.012937	-0.002394	-0.007998
	DS* (-1 < x_f, y_f, z_f < 2)	0.000541	-0.000702	-0.007234	0.012995	-0.002211	-0.008138
H2	Single molecule	-1.828232	-2.207823	-1.787421	0.139726	0.014358	-0.041136
	ES*	-0.011649	0.009775	-0.012831	-0.005613	0.000956	0.003869
	DS* (-4 < x_f, y_f, z_f < 5)	-0.011650	0.009777	-0.012831	-0.005600	0.000960	0.003864
	DS* (-3 < x_f, y_f, z_f < 4)	-0.011651	0.009777	-0.012831	-0.005592	0.000962	0.003860
	DS* (-2 < x_f, y_f, z_f < 3)	-0.011652	0.009766	-0.012819	-0.005572	0.000973	0.003833
	DS* (-1 < x_f, y_f, z_f < 2)	-0.011690	0.009600	-0.012615	-0.005502	0.001069	0.003418
H3	Single molecule	-1.791098	-1.796326	-2.234566	0.012501	0.063898	-0.094410
	ES*	0.001407	-0.015006	0.008029	-0.004955	-0.006869	0.003853
	DS* (-4 < x_f, y_f, z_f < 5)	0.001406	-0.015005	0.008029	-0.004942	-0.006866	0.003847
	DS* (-3 < x_f, y_f, z_f < 4)	0.001405	-0.015004	0.008029	-0.004934	-0.006863	0.003843
	DS* (-2 < x_f, y_f, z_f < 3)	0.001405	-0.015000	0.008025	-0.004913	-0.006852	0.003822
	DS* (-1 < x_f, y_f, z_f < 2)	0.001439	-0.014955	0.007946	-0.004805	-0.006707	0.003565

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C1	Single molecule	-533.834635	-533.996504	-534.403321	0.043393	0.098917	0.110398
	ES*	-0.001026	-0.002807	0.003347	-0.002286	0.001495	-0.003769
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001028	-0.002806	0.003346	-0.002272	0.001499	-0.003774
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001029	-0.002805	0.003346	-0.002264	0.001501	-0.003778
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001031	-0.002800	0.003344	-0.002242	0.001510	-0.003794
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001033	-0.002743	0.003289	-0.002164	0.001592	-0.003947
C2	Single molecule	-534.277109	-533.956330	-534.042962	0.041147	-0.172965	0.033264
	ES*	-0.000830	-0.000361	0.001100	0.000321	0.000878	-0.000430
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000831	-0.000359	0.001100	0.000334	0.000881	-0.000436
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000832	-0.000358	0.001100	0.000343	0.000883	-0.000440
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000834	-0.000363	0.001107	0.000364	0.000891	-0.000456
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000831	-0.000480	0.001221	0.000448	0.000959	-0.000649
H4	Single molecule	-2.129713	-2.130909	-2.014163	-0.173402	0.089330	0.104644
	ES*	-0.000688	-0.000228	0.000503	0.001381	-0.000962	0.005767
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000690	-0.000226	0.000503	0.001394	-0.000959	0.005762
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000691	-0.000226	0.000503	0.001403	-0.000956	0.005758
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000690	-0.000233	0.000510	0.001426	-0.000948	0.005735
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000651	-0.000376	0.000614	0.001545	-0.000862	0.005408
C3	Single molecule	-534.156572	-534.158993	-534.186547	0.034236	0.014573	-0.018163
	ES*	-0.000699	0.000499	0.000161	0.000847	0.002167	-0.002546
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000700	0.000500	0.000161	0.000861	0.002170	-0.002551
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000701	0.000501	0.000161	0.000869	0.002173	-0.002555
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000704	0.000491	0.000173	0.000890	0.002177	-0.002559
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000710	0.000239	0.000431	0.000962	0.002164	-0.002540
H5	Single molecule	-2.119200	-2.185548	-1.952032	0.211316	0.016916	-0.025734
	ES*	-0.001366	-0.000691	0.001537	0.001706	0.001634	-0.003546
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001368	-0.000690	0.001537	0.001719	0.001637	-0.003551
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001368	-0.000690	0.001538	0.001728	0.001639	-0.003555
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001371	-0.000710	0.001560	0.001747	0.001643	-0.003556
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001359	-0.001202	0.002040	0.001782	0.001618	-0.003492
C4	Single molecule	-533.549388	-533.548641	-533.549485	0.004872	0.005099	0.006014
	ES*	-0.000332	0.000097	0.000186	0.000364	0.002397	-0.003069
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000333	0.000098	0.000185	0.000378	0.002400	-0.003075
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000334	0.000099	0.000186	0.000386	0.002402	-0.003078
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000335	0.000088	0.000198	0.000409	0.002403	-0.003077
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000329	-0.000181	0.000461	0.000528	0.002333	-0.002940
H6	Single molecule	-2.054819	-2.306259	-2.118902	-0.153315	0.093401	0.212480
	ES*	0.000675	-0.002442	0.001415	0.000926	0.001813	-0.004874
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000674	-0.002440	0.001415	0.000940	0.001816	-0.004880
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000673	-0.002441	0.001416	0.000949	0.001818	-0.004883
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000676	-0.002466	0.001439	0.000974	0.001818	-0.004885
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000690	-0.002961	0.001919	0.001173	0.001743	-0.004836

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-2.226504	-2.275311	-1.979771	0.263165	0.010882	-0.012718
	ES*	0.000266	0.001041	-0.001750	-0.000040	0.003258	-0.002268
	DS* (-4 < x_f, y_f, z_f < 5)	0.000265	0.001042	-0.001750	-0.000027	0.003262	-0.002274
	DS* (-3 < x_f, y_f, z_f < 4)	0.000264	0.001043	-0.001750	-0.000018	0.003263	-0.002277
	DS* (-2 < x_f, y_f, z_f < 3)	0.000263	0.001040	-0.001745	0.000005	0.003263	-0.002280
	DS* (-1 < x_f, y_f, z_f < 2)	0.000280	0.000913	-0.001635	0.000092	0.003187	-0.002210
H8	Single molecule	-1.994775	-2.014491	-2.469959	0.016742	0.064263	-0.134320
	ES*	-0.000331	-0.000874	0.000887	0.000652	0.002201	-0.002385
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000332	-0.000872	0.000887	0.000665	0.002205	-0.002390
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000333	-0.000871	0.000887	0.000674	0.002207	-0.002393
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000336	-0.000877	0.000895	0.000695	0.002207	-0.002382
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000360	-0.001040	0.001082	0.000803	0.002106	-0.002040
C5	Single molecule	-533.550491	-533.549920	-533.543763	0.004170	-0.008975	-0.005769
	ES*	-0.000149	-0.000839	0.000823	0.000632	0.002419	-0.001528
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000150	-0.000838	0.000823	0.000645	0.002422	-0.001534
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000152	-0.000836	0.000823	0.000654	0.002424	-0.001537
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000158	-0.000836	0.000829	0.000672	0.002427	-0.001539
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000219	-0.000900	0.000954	0.000712	0.002380	-0.001443
H9	Single molecule	-2.348359	-2.039933	-2.092675	-0.147903	-0.202332	-0.069334
	ES*	-0.000652	-0.003736	0.002262	0.002171	0.005576	-0.001011
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000653	-0.003734	0.002262	0.002184	0.005579	-0.001016
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000655	-0.003733	0.002262	0.002192	0.005581	-0.001020
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000666	-0.003731	0.002271	0.002209	0.005585	-0.001024
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000793	-0.003768	0.002435	0.002218	0.005547	-0.000969
H10	Single molecule	-2.004086	-2.023367	-2.451107	0.029811	0.110359	-0.133089
	ES*	-0.000767	-0.001478	0.001923	0.000337	0.001052	-0.001319
	DS* (-4 < x_f, y_f, z_f < 5)	-0.000768	-0.001477	0.001922	0.000350	0.001056	-0.001325
	DS* (-3 < x_f, y_f, z_f < 4)	-0.000770	-0.001476	0.001922	0.000359	0.001058	-0.001328
	DS* (-2 < x_f, y_f, z_f < 3)	-0.000775	-0.001474	0.001926	0.000377	0.001058	-0.001328
	DS* (-1 < x_f, y_f, z_f < 2)	-0.000812	-0.001529	0.002018	0.000419	0.000978	-0.001170
H11	Single molecule	-2.217877	-2.284165	-1.979909	0.263791	-0.010636	0.016940
	ES*	0.000557	-0.000577	-0.000302	-0.000018	0.001769	-0.001847
	DS* (-4 < x_f, y_f, z_f < 5)	0.000556	-0.000575	-0.000302	-0.000004	0.001772	-0.001853
	DS* (-3 < x_f, y_f, z_f < 4)	0.000554	-0.000574	-0.000302	0.000004	0.001774	-0.001856
	DS* (-2 < x_f, y_f, z_f < 3)	0.000549	-0.000570	-0.000300	0.000024	0.001777	-0.001858
	DS* (-1 < x_f, y_f, z_f < 2)	0.000496	-0.000555	-0.000263	0.000074	0.001737	-0.001749

Table S33 Elements of the traceless electric field gradient (EFG) tensors $\nabla\mathcal{E}_{\alpha\beta}$ (atomic units) at the locations of the nuclei of the central **VAL** molecule in the crystal from different calculations. * Both the Ewald (ES) and direct summation (DS) calculations exclude contributions of the central molecule, thus indicating the effect of the crystal environment.

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
O1	Single molecule	0.482400	0.150252	-0.632651	-1.297561	-0.124875	-0.024197
	ES*	0.005190	-0.016357	0.011166	0.009007	-0.003669	-0.002889
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.005188	-0.016355	0.011166	0.009027	-0.003664	-0.002897
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.005187	-0.016353	0.011166	0.009040	-0.003660	-0.002903
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.005181	-0.016339	0.011158	0.009072	-0.003643	-0.002929
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.005114	-0.016112	0.010998	0.009168	-0.003448	-0.003200
O2	Single molecule	-0.947822	1.443853	-0.496031	0.428026	0.042813	0.502718
	ES*	0.000091	-0.000944	0.000853	-0.017553	0.010570	-0.007073
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000089	-0.000942	0.000853	-0.017533	0.010575	-0.007081
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000088	-0.000940	0.000852	-0.017520	0.010579	-0.007087
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000088	-0.000931	0.000843	-0.017486	0.010590	-0.007109
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000156	-0.000809	0.000653	-0.017343	0.010693	-0.007328
N1	Single molecule	0.058496	-0.040034	-0.018463	-0.012880	0.075147	-0.007577
	ES*	-0.001243	0.000540	0.000703	0.000902	-0.001415	0.000325
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001245	0.000542	0.000703	0.000922	-0.001410	0.000317
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001247	0.000543	0.000703	0.000934	-0.001406	0.000311
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001250	0.000539	0.000711	0.000964	-0.001390	0.000282
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001284	0.000430	0.000854	0.001084	-0.001197	-0.000096
H1	Single molecule	-0.125655	-0.006587	0.132242	-0.311210	0.190758	0.163163
	ES*	0.004653	0.002761	-0.007414	0.019347	-0.003621	-0.011963
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004651	0.002763	-0.007414	0.019367	-0.003616	-0.011971
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004649	0.002765	-0.007414	0.019379	-0.003612	-0.011976
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004639	0.002763	-0.007402	0.019406	-0.003592	-0.011998
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004509	0.002645	-0.007153	0.019493	-0.003316	-0.012207
H2	Single molecule	0.169390	-0.399996	0.230607	0.209588	0.021537	-0.061704
	ES*	-0.010121	0.022015	-0.011894	-0.008419	0.001435	0.005804
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.010123	0.022017	-0.011895	-0.008400	0.001440	0.005796
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.010124	0.022018	-0.011894	-0.008387	0.001443	0.005790
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.010126	0.022002	-0.011876	-0.008358	0.001459	0.005750
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.010183	0.021753	-0.011570	-0.008253	0.001604	0.005127
H3	Single molecule	0.224349	0.216506	-0.440854	0.018752	0.095847	-0.141616
	ES*	0.004896	-0.019724	0.014828	-0.007433	-0.010303	0.005779
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.004894	-0.019722	0.014828	-0.007413	-0.010298	0.005771
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.004893	-0.019721	0.014828	-0.007401	-0.010295	0.005765
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.004893	-0.019716	0.014823	-0.007369	-0.010277	0.005734
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.004943	-0.019647	0.014704	-0.007207	-0.010060	0.005348

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
C1	Single molecule	0.365277	0.122474	-0.487751	0.065090	0.148376	0.165597
	ES*	-0.001296	-0.003967	0.005263	-0.003428	0.002243	-0.005653
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001298	-0.003965	0.005263	-0.003409	0.002248	-0.005662
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001300	-0.003963	0.005263	-0.003395	0.002251	-0.005667
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001303	-0.003956	0.005259	-0.003363	0.002264	-0.005690
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001307	-0.003871	0.005177	-0.003246	0.002388	-0.005921
C2	Single molecule	-0.277463	0.203705	0.073757	0.061721	-0.259448	0.049897
	ES*	-0.001199	-0.000496	0.001695	0.000481	0.001317	-0.000646
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001202	-0.000494	0.001695	0.000501	0.001322	-0.000654
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001203	-0.000493	0.001696	0.000514	0.001325	-0.000660
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001205	-0.000500	0.001705	0.000546	0.001337	-0.000684
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001202	-0.000675	0.001877	0.000673	0.001438	-0.000974
H4	Single molecule	-0.057177	-0.058971	0.116148	-0.260103	0.133996	0.156967
	ES*	-0.000826	-0.000135	0.000961	0.002072	-0.001443	0.008651
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000828	-0.000133	0.000961	0.002092	-0.001438	0.008642
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000829	-0.000132	0.000962	0.002105	-0.001435	0.008636
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000828	-0.000143	0.000972	0.002140	-0.001422	0.008602
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000769	-0.000358	0.001128	0.002317	-0.001293	0.008112
C3	Single molecule	0.016198	0.012566	-0.028765	0.051353	0.021860	-0.027245
	ES*	-0.001029	0.000768	0.000261	0.001271	0.003251	-0.003819
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001031	0.000770	0.000261	0.001291	0.003256	-0.003827
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001032	0.000771	0.000261	0.001304	0.003259	-0.003832
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001037	0.000757	0.000280	0.001335	0.003265	-0.003839
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001045	0.000379	0.000666	0.001443	0.003246	-0.003810
H5	Single molecule	-0.050410	-0.149932	0.200342	0.316974	0.025375	-0.038601
	ES*	-0.001789	-0.000777	0.002566	0.002559	0.002451	-0.005319
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.001791	-0.000774	0.002566	0.002579	0.002456	-0.005327
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.001792	-0.000775	0.002567	0.002592	0.002459	-0.005332
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001796	-0.000805	0.002601	0.002621	0.002465	-0.005334
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001778	-0.001543	0.003320	0.002673	0.002427	-0.005238
C4	Single molecule	-0.000325	0.000796	-0.000470	0.007307	0.007648	0.009020
	ES*	-0.000473	0.000170	0.000303	0.000546	0.003595	-0.004604
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000475	0.000172	0.000303	0.000566	0.003600	-0.004612
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000476	0.000173	0.000303	0.000580	0.003603	-0.004617
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000478	0.000156	0.000322	0.000613	0.003604	-0.004615
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000469	-0.000247	0.000716	0.000792	0.003499	-0.004410
H6	Single molecule	0.157762	-0.219399	0.061637	-0.229972	0.140102	0.318720
	ES*	0.001189	-0.003487	0.002298	0.001390	0.002719	-0.007311
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.001187	-0.003485	0.002298	0.001410	0.002724	-0.007319
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.001186	-0.003485	0.002299	0.001424	0.002727	-0.007324
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.001190	-0.003524	0.002334	0.001461	0.002728	-0.007327
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.001211	-0.004265	0.003054	0.001760	0.002614	-0.007253

ATOM	CALCULATION	XX	YY	ZZ	XY	XZ	YZ
H7	Single molecule	-0.098962	-0.172174	0.271136	0.394747	0.016324	-0.019076
	ES*	0.000621	0.001783	-0.002403	-0.000060	0.004887	-0.003402
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000618	0.001785	-0.002403	-0.000040	0.004892	-0.003411
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000617	0.001786	-0.002403	-0.000027	0.004895	-0.003416
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000615	0.001781	-0.002396	0.000007	0.004895	-0.003420
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000641	0.001590	-0.002231	0.000138	0.004780	-0.003315
H8	Single molecule	0.247450	0.217876	-0.465326	0.025114	0.096394	-0.201479
	ES*	-0.000337	-0.001152	0.001490	0.000977	0.003302	-0.003577
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000340	-0.001150	0.001489	0.000997	0.003307	-0.003585
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000341	-0.001149	0.001489	0.001011	0.003310	-0.003589
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000345	-0.001156	0.001502	0.001043	0.003310	-0.003573
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000381	-0.001401	0.001782	0.001204	0.003160	-0.003060
C5	Single molecule	-0.003649	-0.002793	0.006442	0.006255	-0.013463	-0.008654
	ES*	-0.000141	-0.001176	0.001317	0.000948	0.003628	-0.002292
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000143	-0.001174	0.001317	0.000968	0.003633	-0.002301
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000145	-0.001172	0.001317	0.000980	0.003636	-0.002306
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.000155	-0.001172	0.001326	0.001009	0.003640	-0.002309
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000246	-0.001268	0.001514	0.001067	0.003571	-0.002165
H9	Single molecule	-0.282056	0.180584	0.101471	-0.221854	-0.303499	-0.104001
	ES*	0.000085	-0.004541	0.004456	0.003257	0.008363	-0.001516
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000083	-0.004539	0.004456	0.003276	0.008368	-0.001524
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000080	-0.004537	0.004456	0.003289	0.008372	-0.001529
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000064	-0.004533	0.004469	0.003314	0.008377	-0.001535
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.000127	-0.004588	0.004716	0.003328	0.008321	-0.001453
H10	Single molecule	0.233151	0.204230	-0.437381	0.044716	0.165538	-0.199634
	ES*	-0.000989	-0.002056	0.003045	0.000506	0.001578	-0.001979
	DS* ($-4 < x_f, y_f, z_f < 5$)	-0.000991	-0.002054	0.003045	0.000526	0.001583	-0.001987
	DS* ($-3 < x_f, y_f, z_f < 4$)	-0.000993	-0.002052	0.003045	0.000538	0.001586	-0.001992
	DS* ($-2 < x_f, y_f, z_f < 3$)	-0.001001	-0.002050	0.003051	0.000566	0.001587	-0.001991
	DS* ($-1 < x_f, y_f, z_f < 2$)	-0.001057	-0.002132	0.003188	0.000629	0.001467	-0.001756
H11	Single molecule	-0.085839	-0.185272	0.271111	0.395687	-0.015954	0.025410
	ES*	0.000996	-0.000705	-0.000292	-0.000026	0.002653	-0.002771
	DS* ($-4 < x_f, y_f, z_f < 5$)	0.000994	-0.000702	-0.000292	-0.000006	0.002658	-0.002779
	DS* ($-3 < x_f, y_f, z_f < 4$)	0.000992	-0.000700	-0.000292	0.000007	0.002661	-0.002784
	DS* ($-2 < x_f, y_f, z_f < 3$)	0.000984	-0.000694	-0.000289	0.000036	0.002665	-0.002786
	DS* ($-1 < x_f, y_f, z_f < 2$)	0.000905	-0.000671	-0.000233	0.000111	0.002605	-0.002623

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