

## Supplementary information

**Table S1** – GED data analysis parameters

Dataset	1	2
$R_G$	3.04%	12.75%
$R_D$	2.06%	8.79%
Scale Factor, $k$	0.713(4)	0.738(14)
Correlation Parameter	0.3731	0.4944
$\Delta s / \text{nm}^{-1}$	2	2
$s_{\text{min}} / \text{nm}^{-1}$	22	80
$s_{\text{w1}} / \text{nm}^{-1}$	42	120
$s_{\text{w2}} / \text{nm}^{-1}$	126	300
$s_{\text{max}} / \text{nm}^{-1}$	146	340
Camera Distance / mm	501.88	252.78
Electron wavelength / Å	0.0487	0.0485

**Table S2** – GED least-squares correlation matrix.<sup>a</sup>

	$p_8$	$u_{22}$	$u_{101}$	$u_{121}$	$u_{221}$	$k_1$	$k_2$
$p_1$	57						
$p_2$	52						
$p_3$	-57						
$p_7$		-50					
$p_{12}$			53		69		
$p_{13}$				57			
$u_{20}$						57	59
$u_{101}$					55		

<sup>a</sup> Parameters ( $p$ ) are given in Table 3, amplitudes of vibration ( $u$ ) are as defined in Table S3 and  $k_1$  and  $k_2$  are the scale factors for data sets 1 and 2, respectively.

**Table S3** – Refined interatomic distances ( $r_a$ ), root-mean-squared amplitudes of vibration ( $u$ ) and distance corrections for perpendicular motion ( $k_{h1}$ ).

	Atom pair	$r_a$	$u$ (GED)	$k_{h1}$	$u$ (B3LYP/ 6-311G*)
u14	C(10)-F(14)	1.332(1)	0.044(1)	0.001	0.045
u8	C(3)-F(7)	1.332(1)	0.044( Tied to u14)	0.001	0.045
u20	C(17)-F(21)	1.332(1)	0.044( Tied to u14)	0.001	0.045
u9	C(3)-F(8)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u15	C(10)-F(15)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u19	C(17)-F(20)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u7	C(3)-F(6)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u21	C(17)-F(22)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u13	C(10)-F(13)	1.332(1)	0.045( Tied to u14)	0.001	0.045
u5	C(2)-F(4)	1.344(2)	0.046( Tied to u14)	0.001	0.046
u17	C(16)-F(18)	1.344(2)	0.046( Tied to u14)	0.001	0.046
u11	C(9)-F(11)	1.344(2)	0.046( Tied to u14)	0.001	0.046
u18	C(16)-F(19)	1.351(2)	0.046( Tied to u14)	0.001	0.046
u12	C(9)-F(12)	1.351(2)	0.046( Tied to u14)	0.001	0.046

u6	C(2)-F(5)	1.351(2)	0.046( Tied to u14)	0.001	0.046
u16	C(16)-C(17)	1.533(3)	0.051( Tied to u14)	0.002	0.052
u4	C(2)-C(3)	1.533(3)	0.051( Tied to u14)	0.002	0.052
u10	C(9)-C(10)	1.533(3)	0.051( Tied to u14)	0.002	0.052
u2	P(1)-C(9)	1.904(3)	0.063( Tied to u1)	0.001	0.057
u1	P(1)-C(2)	1.904(3)	0.063(3)	0.001	0.057
u3	P(1)-C(16)	1.904(3)	0.063( Tied to u1)	0.001	0.057
u124	F(7)...F(8)	2.154(1)	0.062(1)	-0.001	0.056
u109	F(6)...F(8)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u194	F(13)...F(15)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u230	F(20)...F(22)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u193	F(13)...F(14)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u202	F(14)...F(15)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u108	F(6)...F(7)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u231	F(21)...F(22)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u229	F(20)...F(21)	2.154(1)	0.062( Tied to u124)	-0.001	0.056
u222	F(18)...F(19)	2.179(3)	0.064( Tied to u124)	-0.001	0.058
u172	F(11)...F(12)	2.179(3)	0.064( Tied to u124)	-0.001	0.058
u73	F(4)...F(5)	2.179(3)	0.064( Tied to u124)	-0.001	0.058
u164	C(10)...F(12)	2.291(6)	0.073( Tied to u124)	-0.001	0.066
u58	C(3)...F(5)	2.291(6)	0.073( Tied to u124)	-0.001	0.066
u221	C(17)...F(19)	2.291(6)	0.073( Tied to u124)	-0.001	0.066
u163	C(10)...F(11)	2.334(6)	0.074( Tied to u124)	-0.001	0.067
u220	C(17)...F(18)	2.334(6)	0.074( Tied to u124)	-0.001	0.067
u57	C(3)...F(4)	2.334(6)	0.074( Tied to u124)	-0.001	0.067
u40	C(2)...F(6)	2.359(2)	0.076( Tied to u124)	-0.001	0.069
u153	C(9)...F(13)	2.359(2)	0.076( Tied to u124)	-0.001	0.069
u217	C(16)...F(20)	2.359(2)	0.076( Tied to u124)	-0.001	0.069
u155	C(9)...F(15)	2.359(2)	0.074( Tied to u124)	-0.001	0.067
u42	C(2)...F(8)	2.359(2)	0.074( Tied to u124)	-0.001	0.067
u219	C(16)...F(22)	2.359(2)	0.074( Tied to u124)	-0.001	0.067
u154	C(9)...F(14)	2.360(2)	0.074( Tied to u124)	0.000	0.067
u41	C(2)...F(7)	2.360(2)	0.074( Tied to u124)	0.000	0.067
u218	C(16)...F(22)	2.360(2)	0.074( Tied to u124)	0.000	0.067
u36	P(1)...F(19)	2.650(5)	0.097(2)	-0.001	0.080
u24	P(1)...F(5)	2.650(5)	0.097( Tied to u36)	-0.001	0.080
u30	P(1)...F(12)	2.650(5)	0.097( Tied to u36)	-0.001	0.080
u184	F(12)...F(14)	2.669(10)	0.192( Tied to u36)	0.001	0.159
u227	F(19)...F(21)	2.669(10)	0.192( Tied to u36)	0.001	0.159
u92	F(5)...F(7)	2.669(10)	0.192( Tied to u36)	0.001	0.159
u93	F(5)...F(8)	2.681(13)	0.164( Tied to u36)	0.004	0.135
u228	F(19)...F(22)	2.681(13)	0.164( Tied to u36)	0.004	0.135
u185	F(12)...F(15)	2.681(13)	0.164( Tied to u36)	0.004	0.135
u224	F(18)...F(21)	2.699(10)	0.160( Tied to u36)	0.005	0.132
u174	F(11)...F(14)	2.699(10)	0.160( Tied to u36)	0.005	0.132
u75	F(4)...F(7)	2.699(10)	0.160( Tied to u36)	0.005	0.132
u105	F(5)...F(20)	2.720(14)	0.238( Tied to u36)	0.044	0.196
u198	F(13)...F(19)	2.720(14)	0.238( Tied to u36)	0.044	0.196
u113	F(6)...F(12)	2.720(14)	0.238( Tied to u36)	0.044	0.196

u23	P(1)...F(4)	2.721(5)	0.086( Tied to u36)	-0.001	0.071
u35	P(1)...F(18)	2.721(5)	0.086( Tied to u36)	-0.001	0.071
u29	P(1)...F(11)	2.721(5)	0.086( Tied to u36)	-0.001	0.071
u179	F(11)...F(19)	2.727(14)	0.213( Tied to u36)	0.011	0.176
u80	F(4)...F(12)	2.727(14)	0.213( Tied to u36)	0.011	0.176
u103	F(5)...F(18)	2.727(14)	0.213( Tied to u36)	0.011	0.176
u74	F(4)...F(6)	2.768(13)	0.177( Tied to u36)	0.001	0.146
u173	F(11)...F(13)	2.768(13)	0.177( Tied to u36)	0.001	0.146
u223	F(18)...F(20)	2.768(13)	0.177( Tied to u36)	0.001	0.146
u34	P(1)...C(17)	2.882(7)	0.100( Tied to u36)	-0.002	0.083
u22	P(1)...C(3)	2.882(7)	0.100( Tied to u36)	-0.002	0.083
u28	P(1)...C(10)	2.882(7)	0.100( Tied to u36)	-0.002	0.083
u176	F(11)...C(16)	2.911(7)	0.158( Tied to u36)	0.005	0.130
u77	F(4)...C(9)	2.911(7)	0.158( Tied to u36)	0.005	0.130
u52	C(2)...F(18)	2.911(7)	0.158( Tied to u36)	0.005	0.130
u156	C(9)...C(16)	2.915(5)	0.105( Tied to u36)	0.000	0.087
u50	C(2)...C(16)	2.915(5)	0.105( Tied to u36)	0.000	0.087
u43	C(2)...C(9)	2.915(5)	0.105( Tied to u36)	0.000	0.087
u178	F(11)...F(18)	2.942(17)	0.264( Tied to u36)	0.009	0.218
u86	F(4)...F(18)	2.942(17)	0.264( Tied to u36)	0.009	0.218
u79	F(4)...F(11)	2.942(17)	0.264( Tied to u36)	0.009	0.218
u159	C(9)...F(19)	2.948(8)	0.147( Tied to u36)	0.004	0.122
u46	C(2)...F(12)	2.948(8)	0.147( Tied to u36)	0.004	0.122
u101	F(5)...C(16)	2.948(8)	0.147( Tied to u36)	0.004	0.122
u27	P(1)...F(8)	3.150(13)	0.198( Tied to u36)	0.002	0.163
u33	P(1)...F(15)	3.150(13)	0.198( Tied to u36)	0.002	0.163
u39	P(1)...F(22)	3.150(13)	0.198( Tied to u36)	0.002	0.163
u31	P(1)...F(13)	3.189(12)	0.234( Tied to u36)	0.001	0.193
u37	P(1)...F(20)	3.189(12)	0.234( Tied to u36)	0.001	0.193
u25	P(1)...F(6)	3.189(12)	0.234( Tied to u36)	0.001	0.193
u168	C(10)...F(19)	3.360(8)	0.180( Tied to u226)	0.007	0.154
u102	F(5)...C(17)	3.360(8)	0.180( Tied to u226)	0.007	0.154
u62	C(3)...F(12)	3.360(8)	0.180( Tied to u226)	0.007	0.154
u158	C(9)...F(18)	3.388(10)	0.178( Tied to u226)	-0.002	0.151
u45	C(2)...F(11)	3.388(10)	0.178( Tied to u226)	-0.002	0.151
u84	F(4)...C(16)	3.388(10)	0.178( Tied to u226)	-0.002	0.151
u183	F(12)...F(13)	3.460(4)	0.076( Tied to u226)	-0.014	0.065
u226	F(19)...F(20)	3.460(4)	0.076(2)	-0.014	0.065
u91	F(5)...F(6)	3.460(4)	0.076( Tied to u226)	-0.014	0.065
u225	F(18)...F(22)	3.488(4)	0.077( Tied to u226)	-0.013	0.066
u175	F(11)...F(15)	3.488(4)	0.077( Tied to u226)	-0.012	0.066
u76	F(4)...F(8)	3.488(4)	0.077( Tied to u226)	-0.012	0.066
u54	C(2)...F(20)	3.521(15)	0.204( Tied to u226)	0.017	0.174
u195	F(13)...C(16)	3.521(15)	0.204( Tied to u226)	0.017	0.174
u110	F(6)...C(9)	3.521(15)	0.204( Tied to u226)	0.017	0.174
u51	C(2)...C(17)	3.785(9)	0.136(Tied to u38)	-0.003	0.108
u59	C(3)...C(9)	3.785(9)	0.136(Tied to u38)	-0.003	0.108
u165	C(10)...C(16)	3.785(9)	0.136(Tied to u38)	-0.003	0.108
u186	F(12)...C(16)	4.014(5)	0.118(Tied to u38)	-0.006	0.094

u53	C(2)...F(19)	4.014(5)	0.118(Tied to u38)	-0.006	0.094
u94	F(5)...C(9)	4.014(5)	0.118(Tied to u38)	-0.006	0.094
u32	P(1)...F(14)	4.059(5)	0.096(Tied to u38)	-0.017	0.077
u38	P(1)...F(21)	4.059(5)	0.096(4)	-0.017	0.077
u26	P(1)...F(7)	4.059(5)	0.096(Tied to u38)	-0.017	0.076
u107	F(5)...F(22)	4.216(16)	0.260(Tied to u189)	-0.014	0.212
u142	F(8)...F(12)	4.216(16)	0.260(Tied to u189)	-0.014	0.212
u213	F(15)...F(19)	4.216(16)	0.260(Tied to u189)	-0.013	0.212
u189	F(12)...F(19)	4.252(10)	0.150(4)	-0.005	0.122
u104	F(5)...F(19)	4.252(10)	0.150(Tied to u189)	-0.005	0.122
u97	F(5)...F(12)	4.252(10)	0.150(Tied to u189)	-0.005	0.122
u200	F(13)...F(22)	4.261(22)	0.330(Tied to u189)	0.005	0.269
u150	F(8)...F(20)	4.278(23)	0.432(Tied to u189)	0.040	0.352
u201	F(13)...F(22)	4.278(23)	0.432(Tied to u189)	0.040	0.352
u116	F(6)...F(15)	4.278(23)	0.432(Tied to u189)	0.040	0.352
u206	F(14)...F(19)	4.282(14)	0.292(Tied to u189)	-0.003	0.238
u128	F(7)...F(12)	4.282(14)	0.292(Tied to u189)	-0.003	0.238
u106	F(5)...F(21)	4.282(14)	0.292(Tied to u189)	-0.003	0.238
u188	F(12)...F(18)	4.285(8)	0.216(Tied to u189)	-0.005	0.176
u87	F(4)...F(19)	4.285(8)	0.216(Tied to u189)	-0.005	0.176
u96	F(5)...F(11)	4.285(8)	0.216(Tied to u189)	-0.005	0.176
u157	C(9)...C(17)	4.299(6)	0.113(Tied to u189)	-0.008	0.092
u44	C(2)...C(10)	4.299(6)	0.113(Tied to u189)	-0.008	0.092
u66	C(3)...C(16)	4.299(6)	0.113(Tied to u189)	-0.008	0.092
u177	F(11)...C(17)	4.426(7)	0.161(Tied to u189)	-0.006	0.131
u68	C(3)...F(18)	4.426(7)	0.161(Tied to u189)	-0.006	0.131
u78	F(4)...C(10)	4.426(7)	0.161(Tied to u189)	-0.006	0.131
u112	F(6)...F(11)	4.427(18)	0.217(Tied to u189)	0.001	0.177
u88	F(4)...F(20)	4.427(18)	0.217(Tied to u189)	0.001	0.177
u197	F(13)...F(18)	4.427(18)	0.217(Tied to u189)	0.001	0.177
u210	F(15)...C(16)	4.453(16)	0.214(Tied to u189)	-0.014	0.174
u56	C(2)...F(22)	4.453(16)	0.214(Tied to u189)	-0.014	0.174
u139	F(8)...C(9)	4.453(16)	0.214(Tied to u189)	-0.014	0.174
u70	C(3)...F(20)	4.514(15)	0.308(Tied to u189)	0.014	0.251
u196	F(13)...C(17)	4.514(15)	0.308(Tied to u189)	0.014	0.251
u111	F(6)...C(10)	4.514(15)	0.308(Tied to u189)	0.014	0.251
u167	C(10)...F(18)	4.535(13)	0.185(Tied to u189)	-0.011	0.151
u85	F(4)...C(17)	4.535(13)	0.185(Tied to u189)	-0.011	0.151
u61	C(3)...F(11)	4.535(13)	0.185(Tied to u189)	-0.011	0.151
u162	C(9)...F(22)	4.576(10)	0.199(Tied to u189)	-0.003	0.162
u49	C(2)...F(15)	4.576(10)	0.199(Tied to u189)	-0.003	0.162
u146	F(8)...C(16)	4.576(10)	0.199(Tied to u189)	-0.003	0.162
u203	F(14)...C(16)	4.843(11)	0.205(Tied to u83)	-0.017	0.163
u125	F(7)...C(9)	4.843(11)	0.205(Tied to u83)	-0.017	0.163
u55	C(2)...F(21)	4.843(11)	0.205(Tied to u83)	-0.017	0.163
u160	C(9)...F(20)	4.886(9)	0.191(Tied to u83)	-0.013	0.152
u47	C(2)...F(13)	4.886(9)	0.191(Tied to u83)	-0.013	0.152
u117	F(6)...C(16)	4.886(9)	0.191(Tied to u83)	-0.013	0.152
u147	F(8)...C(17)	4.897(16)	0.304(Tied to u83)	0.006	0.242

u171	C(10)...F(22)	4.897(16)	0.304(Tied to u83)	0.006	0.242
u65	C(3)...F(15)	4.897(16)	0.304(Tied to u83)	0.006	0.242
u148	F(8)...F(18)	4.959(10)	0.203(Tied to u83)	-0.008	0.162
u182	F(11)...F(22)	4.959(10)	0.203(Tied to u83)	-0.008	0.162
u83	F(4)...F(15)	4.959(10)	0.203(7)	-0.008	0.162
u166	C(10)...C(17)	4.980(11)	0.187(Tied to u83)	-0.010	0.149
u67	C(3)...C(17)	4.980(11)	0.187(Tied to u83)	-0.010	0.149
u60	C(3)...C(10)	4.980(11)	0.187(Tied to u83)	-0.010	0.149
u181	F(11)...F(21)	5.062(9)	0.224(Tied to u83)	-0.008	0.178
u82	F(4)...F(14)	5.062(9)	0.224(Tied to u83)	-0.008	0.178
u134	F(7)...F(18)	5.062(9)	0.224(Tied to u83)	-0.008	0.178
u215	F(15)...F(22)	5.075(33)	0.307(Tied to u83)	-0.042	0.245
u151	F(8)...F(22)	5.091(33)	0.349(Tied to u83)	-0.021	0.278
u152	F(8)...F(22)	5.103(33)	0.424(Tied to u83)	0.002	0.337
u145	F(8)...F(15)	5.103(33)	0.424(Tied to u83)	0.002	0.337
u216	F(15)...F(22)	5.103(33)	0.424(Tied to u83)	0.002	0.337
u180	F(11)...F(20)	5.121(9)	0.180(Tied to u83)	-0.014	0.143
u119	F(6)...F(18)	5.121(9)	0.180(Tied to u83)	-0.014	0.143
u81	F(4)...F(13)	5.121(9)	0.180(Tied to u83)	-0.014	0.143
u136	F(7)...F(20)	5.198(13)	0.339(Tied to u83)	0.005	0.270
u115	F(6)...F(14)	5.199(13)	0.338(Tied to u83)	0.005	0.269
u48	C(2)...F(14)	5.216(5)	0.138(Tied to u83)	-0.020	0.110
u132	F(7)...C(16)	5.216(5)	0.138(Tied to u83)	-0.020	0.110
u161	C(9)...F(21)	5.216(5)	0.138(Tied to u83)	-0.020	0.110
u187	F(12)...C(17)	5.361(6)	0.115(Tied to u83)	-0.015	0.092
u69	C(3)...F(19)	5.361(6)	0.115(Tied to u83)	-0.015	0.092
u95	F(5)...C(10)	5.361(6)	0.115(Tied to u83)	-0.015	0.092
u141	F(8)...F(11)	5.370(13)	0.205(Tied to u83)	-0.023	0.163
u90	F(4)...F(22)	5.370(13)	0.205(Tied to u83)	-0.023	0.163
u212	F(15)...F(18)	5.370(13)	0.205(Tied to u83)	-0.023	0.163
u205	F(14)...F(18)	5.389(18)	0.271(Tied to u83)	-0.018	0.216
u127	F(7)...F(11)	5.389(18)	0.271(Tied to u83)	-0.018	0.216
u89	F(4)...F(21)	5.389(18)	0.271(Tied to u83)	-0.018	0.216
u211	F(15)...C(17)	5.425(23)	0.302(Tied to u83)	-0.018	0.240
u140	F(8)...C(10)	5.425(23)	0.302(Tied to u83)	-0.018	0.240
u72	C(3)...F(22)	5.425(23)	0.302(Tied to u83)	-0.018	0.240
u121	F(6)...F(20)	5.514(21)	0.375(Tied to u83)	-0.011	0.298
u114	F(6)...F(13)	5.514(21)	0.375(Tied to u83)	-0.011	0.298
u199	F(13)...F(20)	5.514(21)	0.374(Tied to u83)	-0.011	0.298
u192	F(12)...F(22)	5.671(12)	0.212(Tied to u83)	-0.014	0.169
u149	F(8)...F(19)	5.671(12)	0.212(Tied to u83)	-0.014	0.169
u100	F(5)...F(15)	5.671(12)	0.212(Tied to u83)	-0.014	0.168
u98	F(5)...F(13)	5.719(9)	0.214(Tied to u83)	-0.014	0.171
u190	F(12)...F(20)	5.719(9)	0.214(Tied to u83)	-0.014	0.171
u120	F(6)...F(19)	5.719(9)	0.214(Tied to u83)	-0.014	0.170
u169	C(10)...F(20)	5.766(14)	0.260(Tied to u83)	-0.023	0.207
u118	F(6)...C(17)	5.766(14)	0.260(Tied to u83)	-0.023	0.207
u63	C(3)...F(13)	5.766(14)	0.260(Tied to u83)	-0.023	0.207
u133	F(7)...C(17)	5.841(11)	0.220(Tied to u83)	-0.025	0.175

u64	C(3)...F(14)	5.841(11)	0.220(Tied to u83)	-0.025	0.175
u170	C(10)...F(21)	5.841(11)	0.220(Tied to u83)	-0.025	0.175
u214	F(15)...F(20)	6.070(18)	0.379(Tied to u135)	-0.024	0.314
u123	F(6)...F(22)	6.070(18)	0.379(Tied to u135)	-0.024	0.314
u143	F(8)...F(13)	6.070(18)	0.379(Tied to u135)	-0.024	0.314
u209	F(14)...F(22)	6.124(15)	0.335(Tied to u135)	-0.021	0.278
u131	F(7)...F(15)	6.124(15)	0.335(Tied to u135)	-0.021	0.278
u204	F(14)...C(17)	6.135(11)	0.230(Tied to u135)	-0.031	0.190
u71	C(3)...F(21)	6.135(11)	0.230(Tied to u135)	-0.031	0.190
u126	F(7)...C(10)	6.135(11)	0.230(Tied to u135)	-0.031	0.190
u135	F(7)...F(19)	6.353(5)	0.130(6)	-0.029	0.108
u99	F(5)...F(14)	6.353(5)	0.130(Tied to u135)	-0.029	0.108
u191	F(12)...F(21)	6.353(5)	0.130(Tied to u135)	-0.029	0.107
u138	F(7)...F(22)	6.442(28)	0.295(Tied to u135)	-0.042	0.245
u144	F(8)...F(14)	6.442(28)	0.295(Tied to u135)	-0.042	0.245
u137	F(7)...F(21)	6.889(6)	0.274(12)	-0.041	0.245
u130	F(7)...F(14)	6.889(6)	0.274(Tied to u137)	-0.041	0.245
u208	F(14)...F(21)	6.889(6)	0.274(Tied to u137)	-0.041	0.245
u207	F(14)...F(20)	6.955(14)	0.222(Tied to u137)	-0.047	0.199
u129	F(7)...F(13)	6.955(14)	0.222(Tied to u137)	-0.047	0.199
u122	F(6)...F(21)	6.955(14)	0.222(Tied to u137)	-0.047	0.199

**Table S4** – Refined GED coordinates. Distances in Å.

	x	y	z
P1	0.0000000	0.0000000	0.0000000
C2	1.6852999	0.0000000	-0.8863891
C3	2.7946011	-0.7175746	-0.1089767
F4	1.6246060	-0.5246484	-2.1231543
F5	2.1006047	1.2812536	-0.9953450
F6	2.4992160	-2.0057386	0.0593764
F7	3.9550054	-0.6419998	-0.7591398
F8	2.9599776	-0.1715183	1.0949481
C9	-0.8426500	-1.4595125	-0.8863891
C10	-2.0187385	-2.0614082	-0.1089767
F11	-1.2666619	-1.1446258	-2.1231543
F12	0.0592957	-2.4598038	-0.9953450
F13	-2.9866286	-1.1615150	0.0593764
F14	-2.5334910	-3.1041351	-0.7591398
F15	-1.6285282	-2.4776566	1.0949481
C16	-0.8426500	1.4595125	-0.8863891
C17	-0.7758629	2.7789828	-0.1089767
F18	-0.3579443	1.6692743	-2.1231543
F19	-2.1599006	1.1785501	-0.9953450
F20	0.4874124	3.1672538	0.0593764
F21	-1.4215148	3.7461349	-0.7591398
F22	-1.3314497	2.6491749	1.0949481

**Table S5** – RI-MP2/TZVPP coordinates and electronic energy for conformer **A**. Distances in Å and energy in Hartrees.

	x	y	z
P	-0.0000061	-0.0000021	-0.5164994
F	1.1281850	2.1711606	0.5380210
F	1.6629546	0.3656623	1.6435738
F	2.5780198	1.4388485	-1.5524132
F	3.7171124	1.3927516	0.2862847
F	3.0950726	-0.4547605	-0.6482565
C	1.4273139	0.8591631	0.4158267
C	2.7438464	0.8022412	-0.3944868
F	-2.4443696	-0.1085534	0.5380215
F	-1.1481669	1.2573389	1.6435720
F	-2.5350878	1.5132156	-1.5524273
F	-3.0647049	2.5227455	0.2862835
F	-1.1536931	2.9077778	-0.6482518
C	-1.4577209	0.8065062	0.4158271
C	-2.0666868	1.9751142	-0.3944934
F	1.3162020	-2.0626091	0.5380107
F	-0.5148140	-1.6230062	1.6435669
F	-0.0429354	-2.9520464	-1.5524180
F	-0.6523881	-3.9154823	0.2862844
F	-1.9413715	-2.4530356	-0.6482520
C	0.0303996	-1.6656730	0.4158237
C	-0.6771600	-2.7773581	-0.3944871
Energy	-2065.0388107730		

**Table S6** – RI-MP2/TZVPP coordinates for conformer **B**. Distances in Å and energy in Hartrees.

	x	y	z
P	0.0000240	0.0001008	0.8170914
C	1.1766129	1.1912098	-0.0880113
C	2.6871353	0.9012806	0.0908956
F	0.9457597	1.3369442	-1.4042900
F	0.9507451	2.3876501	0.5167504
F	3.0780494	-0.0909455	-0.6966527
F	3.3817372	1.9884353	-0.2215522
F	2.9398740	0.5795041	1.3597859
C	0.4431961	-1.6142443	-0.0881548
C	-0.5628874	-2.7776874	0.0910265
F	0.6844689	-1.4872007	-1.4045010
F	1.5924795	-2.0166775	0.5162892
F	-1.6178077	-2.6202645	-0.6962986
F	0.0313899	-3.9226952	-0.2215650
F	-0.9676140	-2.8356867	1.3600078
C	-1.6196879	0.4233668	-0.0880856
C	-2.1243769	1.8762383	0.0909414
F	-1.6302212	0.1507779	-1.4044170
F	-2.5428306	-0.3707579	0.5164057

F	-1.4596992	2.7114232	-0.6953378
F	-3.4128050	1.9340852	-0.2230656
F	-1.9736363	2.2553351	1.3602197
Energy	-2065.0370017636		

**Table S7** – RI-MP2/TZVPP coordinates for conformer **C**. Distances in Å and energy in Hartrees.

	x	y	z
P	0.0484304	-0.0726339	0.8805915
C	-1.8188242	-0.4093354	0.7969827
C	-2.6651872	-0.1995769	-0.4846439
F	-1.9653428	-1.6987699	1.1730089
F	-2.3743138	0.3682607	1.7537293
F	-2.0737712	-0.7412638	-1.5442189
F	-3.8525397	-0.7740703	-0.3183695
F	-2.8512540	1.0952232	-0.7084158
C	0.1345661	1.5885759	-0.0370164
C	1.5302405	2.2477426	0.0315275
F	-0.2377659	1.5750903	-1.3280761
F	-0.7098557	2.4048470	0.6413975
F	2.4103657	1.5421156	-0.6718945
F	1.4674606	3.4755685	-0.4662844
F	1.9437193	2.3150702	1.2950680
C	0.7402296	-1.3082869	-0.4116632
C	2.0419318	-1.9327923	0.1411137
F	-0.1118427	-2.3333032	-0.6093011
F	1.0271909	-0.7551678	-1.6027935
F	1.7755990	-2.6124389	1.2541333
F	2.5708306	-2.7573159	-0.7517468
F	2.9259815	-0.9767837	0.4251525
Energy	-2065.0355282265		

**Table S8** – RI-MP2/TZVPP coordinates for conformer **D**. Distances in Å and energy in Hartrees.

	x	y	z
P	-0.2295815	-0.1686877	0.8119736
C	0.8127343	1.4200311	0.8036077
C	1.3999287	2.0597048	-0.4787016
F	0.0297599	2.3494707	1.3949164
F	1.8587194	1.1782542	1.6272256
F	0.4828010	2.1297979	-1.4376949
F	1.8183430	3.2898535	-0.1971254
F	2.4351104	1.3544242	-0.9166423
C	0.6293983	-1.3499062	-0.4042919
C	1.8524613	-2.0621982	0.2148882
F	-0.2835871	-2.3153476	-0.6702564
F	1.0217683	-0.8125874	-1.5716059
F	1.4995321	-2.6793674	1.3400833



F	2.3264598	-2.9604102	-0.6380099
F	2.8090210	-1.1805861	0.4903692
C	-1.7081883	0.3209786	-0.3031450
C	-2.9949573	-0.3765463	0.1979635
F	-1.9394839	1.6461118	-0.2102711
F	-1.5564723	0.0053121	-1.6013669
F	-3.2623167	0.0155306	1.4418013
F	-4.0168371	-0.0547197	-0.5836831
F	-2.8430709	-1.6983457	0.1892998
Energy	-2065.0358088956		