Electronic Supplementary Information

Note: In all Tables the non-revised output of the XD program (ref. 9) was used. With respect to the significance of the given data we refer to ref. 30, where transferability indices were derived as 0.09 e Å^{-3} and 2.8 e Å^{-5} for the ED's and Laplacians at the bond critical points and 0.7 Å^3 and 0.11 e for the atomic volumes and charges. These quantities can serve as an estimate of the significance of the listed data.

TABLE S1. BOND CRITICAL POINT SEARCH FOR 1a

****

Quantities are in e/Ang^x
using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.600 Angstroms

Bond		ρ	Δρ	Rij	d1	d2	
				Hessian Eigenvalues			ellip
O(1)	-C(22)	2.890	-32.160	1.2382	0.7518	0.4864	
				-25.90	-23.75	17.49	0.09
O(2)	-C(22)	2.355	-29.186	1.3001	0.8126	0.4875	
				-21.83	-19.73	12.37	0.11
C(01)	-C(3)	1.621	-10.210	1.5403	0.7699	0.7704	
				-11.19	-11.12	12.10	0.01
C(01)	-C(1)	1.614	-10.110	1.5378	0.7720	0.7657	
				-11.06	-11.05	12.00	0.00
C(01)	-C(2)	1.616	-10.157	1.5371	0.7714	0.7657	
				-11.09	-11.08	12.01	0.00
C(01)	-C(8)	1.643	-10.035	1.5329	0.7584	0.7745	
				-11.54	-11.09	12.60	0.04
C(02)	-C(6)	1.622	-10.185	1.5352	0.7701	0.7651	
				-11.12	-11.10	12.03	0.00
C(02)	-C(5)	1.618	-10.220	1.5356	0.7711	0.7645	
				-11.12	-11.10	12.00	0.00
C(02)	-C(4)	1.629	-10.343	1.5374	0.7686	0.7688	
				-11.24	-11.19	12.09	0.00
C(02)	-C(7)	1.670	-10.529	1.5237	0.7538	0.7700	
				-11.78	-11.33	12.57	0.04
C(4)	-C(3)	1.681	-11.383	1.5172	0.7586	0.7586	
				-11.71	-11.63	11.96	0.01
C(8)	-C(7)	2.086	-16.516	1.4059	0.7049	0.7010	
				-16.16	-13.37	13.01	0.21
C(8)	-C(9)	2.080	-16.460	1.4042	0.7011	0.7031	
				-16.08	-13.43	13.05	0.20
C(7)	-C(12)	2.106	-16.865	1.3981	0.7002	0.6980	
				-16.39	-13.51	13.04	0.21
C(12)	-C(11)	2.139	-17.775	1.3880	0.6920	0.6961	
				-16.77	-13.79	12.78	0.22
C(11)	-C(10)	2.058	-16.029	1.4129	0.7063	0.7067	
				-15.83	-13.26	13.07	0.19
C(11)	-C(13)	1.696	-10.802	1.5086	0.7638	0.7447	
				-11.94	-11.48	12.62	0.04
C(10)	-C(9)	2.117	-17.249	1.3948	0.6995	0.6952	
				-16.55	-13.61	12.91	0.22
C(10)	-C(14)	1.778	-11.933	1.4905	0.7440	0.7465	

				-12.80	-12.11	12.98	0.06
C(14)	-C(15)	2.329	-19.719	1.3440	0.6741	0.6699	
				-18.43	-14.16	12.87	0.30
C(14)	-C(16)	1.793	-12.230	1.4849	0.7436	0.7413	
				-13.07	-12.12	12.96	0.08
C(16)	-C(17)	2.107	-16.966	1.3997	0.7004	0.6993	
				-16.32	-13.66	13.01	0.20
C(16)	-C(21)	2.103	-16.743	1.4014	0.7020	0.6994	
				-16.33	-13.51	13.10	0.21
C(17)	-C(18)	2.127	-17.612	1.3891	0.6948	0.6943	
				-16.64	-13.79	12.83	0.21
C(18)	-C(19)	2.120	-17.226	1.3955	0.6960	0.6995	
				-16.54	-13.67	12.99	0.21
C(19)	-C(20)	2.114	-17.130	1.3978	0.7005	0.6973	
				-16.40	-13.70	12.97	0.20
C(19)	-C(22)	1.909	-14.870	1.4809	0.7185	0.7624	
				-15.02	-12.99	13.13	0.16
C(20)	-C(21)	2.143	-17.821	1.3858	0.6939	0.6918	
				-16.74	-13.92	12.84	0.20

TABLE S2. BOND CRITICAL POINT SEARCH FOR 1b

****

Quantities are in e/Ang^x
using ANALYTICAL derivatives

Searching internuclear distances between 1.200 and 1.900 Angstroms

Bond		ρ	Δρ	Rij	d1	d2	
				Hessian Eigenvalues			ellip
SI(1)	-C(1)	0.853	-2.945	1.8668	0.7828	1.0840	
				-4.73	-4.56	6.34	0.04
SI(1)	-C(2)	0.836	-2.563	1.8702	0.7833	1.0869	
				-4.48	-4.44	6.35	0.01
SI(1)	-C(3)	0.875	-1.766	1.8750	0.7669	1.1081	
				-4.84	-4.78	7.86	0.01
SI(1)	-C(8)	0.842	-1.992	1.8886	0.7772	1.1114	
				-4.50	-4.48	6.99	0.00
SI(2)	-C(4)	0.868	-1.710	1.8787	0.7679	1.1108	
				-4.79	-4.69	7.77	0.02
SI(2)	-C(5)	0.858	-2.781	1.8632	0.7797	1.0835	
				-4.78	-4.61	6.61	0.04
SI(2)	-C(6)	0.837	-2.549	1.8716	0.7833	1.0882	
				-4.47	-4.43	6.35	0.01
SI(2)	-C(7)	0.849	-2.022	1.8854	0.7760	1.1094	
				-4.61	-4.49	7.08	0.03
O(1)	-C(22)	2.926	-33.371	1.2293	0.7541	0.4752	
				-26.56	-24.37	17.57	0.09
O(2)	-C(22)	2.331	-28.489	1.3070	0.8095	0.4974	
				-21.49	-19.34	12.34	0.11
C(3)	-C(4)	1.576	-9.079	1.5429	0.7712	0.7717	
				-10.39	-10.15	11.46	0.02
C(7)	-C(8)	2.017	-15.746	1.4135	0.7071	0.7064	
				-14.98	-13.10	12.33	0.14
C(7)	-C(12)	2.060	-16.375	1.4052	0.6947	0.7105	
				-15.61	-13.34	12.58	0.17
C(8)	-C(9)	2.055	-16.228	1.4061	0.6956	0.7105	
				-15.54	-13.30	12.61	0.17
C(9)	-C(10)	2.111	-17.171	1.3981	0.6965	0.7017	
				-16.43	-13.61	12.87	0.21
C(10)	-C(11)	2.090	-16.774	1.4031	0.7016	0.7015	
				-16.15	-13.53	12.90	0.19
C(10)	-C(14)	1.757	-11.497	1.4977	0.7476	0.7501	
				-12.35	-12.17	13.03	0.01
C(11)	-C(12)	2.115	-17.269	1.3969	0.7007	0.6962	
				-16.48	-13.64	12.86	0.21
C(11)	-C(13)	1.700	-10.814	1.5081	0.7632	0.7450	
				-11.95	-11.49	12.63	0.04
C(14)	-C(15)	2.349	-20.354	1.3373	0.6717	0.6656	
				-18.68	-14.33	12.66	0.30
C(14)	-C(16)	1.801	-12.401	1.4821	0.7422	0.7399	
				-13.17	-12.17	12.94	0.08
C(16)	-C(17)	2.110	-17.023	1.3989	0.7001	0.6989	
				-16.34	-13.68	13.00	0.19
C(16)	-C(21)	2.097	-16.570	1.4036	0.7027	0.7008	
				-16.25	-13.46	13.14	0.21

C(17)	-C(18)	2.128	-17.626	1.3889	0.6944	0.6945		
				-16.66	-13.80	12.83	0.21	
C(18)	-C(19)	2.128	-17.359	1.3937	0.6955	0.6982		
				-16.60	-13.73	12.97	0.21	
C(19)	-C(20)	2.118	-17.149	1.3972	0.6994	0.6978		
				-16.40	-13.74	12.99	0.19	
C(19)	-C(22)	1.906	-14.816	1.4825	0.7194	0.7631		
				-14.99	-12.96	13.13	0.16	
C(20)	-C(21)	2.131	-17.680	1.3882	0.6940	0.6942		
				-16.69	-13.82	12.83	0.21	

Table S3. Atomic charges q [e] and volumes V [Å^3] for 1a

Atom	q	V_{tot}
O(1)	-0.89794976	17.56412777
O(2)	-1.19123753	19.46640141
C(01)	0.00635142	6.51852219
C(02)	0.01429660	6.43851951
C(6)	-0.09620140	10.19830427
C(5)	-0.10727190	10.37835551
C(4)	-0.05359138	8.42480197
C(3)	-0.05371370	8.08897496
C(1)	-0.09736782	9.83188874
C(2)	-0.10977412	10.01198248
C(8)	-0.05897468	10.31594989
C(7)	-0.04955153	10.73044532
C(12)	-0.05563011	12.83271639
C(11)	-0.05476702	10.63866552
C(10)	-0.04567168	10.63348426
C(9)	-0.06158015	11.84731384
C(13)	-0.03575246	10.29716063
C(14)	-0.03184844	10.43546567
C(15)	-0.08757006	14.93812272
C(16)	-0.04026596	9.68738142
C(17)	-0.06005999	11.38064608
C(18)	-0.05705953	11.14913235
C(19)	-0.02895147	10.05040894
C(20)	-0.05549273	11.30647741
C(21)	-0.06043066	11.91801374
C(22)	1.19991911	7.04391436
H(2)	0.69382834	1.39809458
H(6A)	0.03961157	7.32890732
H(6B)	0.05871383	8.33540344
H(6C)	0.05719853	7.11560086
H(5A)	0.05601229	8.43222601
H(5B)	0.05728322	7.46819232
H(5C)	0.05150929	7.17503775
H(4A)	0.03083914	7.43819803
H(4B)	0.03294499	7.18233751
H(3A)	0.03186794	7.27760906
H(3B)	0.03571053	7.10520178
H(1A)	0.05658007	6.55302684
H(1B)	0.05626853	7.58168708
H(1C)	0.05166024	9.44138041
H(2A)	0.05609267	7.74848813
H(2B)	0.05469296	7.02500522
H(2C)	0.05306518	6.71323639
H(12)	0.07912896	6.89946421
H(9)	0.07880109	6.39277784
H(13A)	0.04735157	9.35702879
H(13B)	0.04845721	6.54731257
H(13C)	0.05277718	8.00903269
H(15A)	0.06530839	7.25943843
H(15B	0.06763278	7.27532230
H(17)	0.07194459	8.21511246
H(18)	0.07942495	6.31687924

H(20)	0.07617832	6.55586817
H(21)	0.07737257	5.61087478
sum:	0.04810996	481.88592156

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Table S4. Atomic charges q [e] and volumes V [Å^3] for 1b

Atom	q	V_{tot}
SI(1)	2.51411721	6.07173315
SI(2)	2.52541435	6.09581202
O(1)	-0.91173913	19.16898170
O(2)	-1.25648897	20.30414029
C(1)	-0.44728476	12.41112457
C(2)	-0.44459804	14.00925937
C(3)	-0.93325116	12.95698125
C(4)	-0.92763427	12.17229287
C(5)	-0.41116295	13.08721856
C(6)	-0.44051163	13.57647308
C(7)	-0.67960802	14.63346140
C(8)	-0.67901573	13.69622503
C(9)	-0.04000437	11.59681688
C(10)	-0.04888320	9.52396645
C(11)	-0.05053347	10.62437392
C(12)	-0.03609365	12.62601360
C(13)	0.00594818	9.38313385
C(14)	-0.03373208	9.60854571
C(15)	-0.07661131	14.13066992
C(16)	-0.03375995	10.12015617
C(17)	-0.04872628	11.76849544
C(18)	-0.03740760	12.65417106
C(19)	-0.02420372	11.28607962
C(20)	-0.02770937	13.05438236
C(21)	-0.02925570	11.60799213
C(22)	1.21428007	7.56935905
H(2)	0.74477329	1.09727193
H(1A)	0.03048719	6.79429831
H(1B)	0.01840063	7.16198248
H(1C)	0.02672631	7.31079553
H(2A)	0.02393344	7.92998630
H(2B)	0.00718340	8.52750469
H(2C)	0.03939396	7.76292468
H(3A)	0.01956134	8.75550677
H(3B)	0.00853807	7.24614334
H(4A)	0.01652283	7.59828669
H(4B)	0.00893792	7.74290906
H(5A)	0.02919923	9.10910734
H(5B)	0.02186689	7.66724185
H(5C)	-0.00321644	8.05395249
H(6A)	0.02929066	8.54742018
H(6B)	0.01437794	9.80485636
H(6C)	0.02902384	7.80526925
H(9)	0.02753265	6.81378756
H(12)	0.03642454	7.05229707
H(13A)	0.03070071	8.61395327
H(13B)	0.02744340	7.10644848
H(13C)	0.01676752	7.93470996
H(15A)	0.04577407	6.46507373
H(15B)	0.03862208	7.05591524
H(17)	0.04709673	8.19842670
H(18)	0.04354435	6.75986183
H(20)	0.03371384	9.68425006

H(21)	0.02583872	8.24080428
sum:	0.08000355	526.57884490

V_{tot} values calculated by integration over the basins enclosed by the zero-flux surfaces of the ED gradient vector field in the crystal according to Bader's formalism.

Tables S5 - S7 for Bexarotene (1a)

Table S5. Atomic coordinates for 1a

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loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

O(1)	O	-0.11509(18)	1.38352(9)	0.55247(5)	0.033	1	2
O(2)	O	0.2163(2)	1.38070(10)	0.49942(6)	0.035	1	2
C(01)	C	-0.2686(2)	0.46476(11)	0.79674(7)	0.019	1	2
C(02)	C	-0.2715(2)	0.71984(11)	0.92573(7)	0.02	1	2
C(6)	C	-0.3867(3)	0.85441(14)	0.94978(10)	0.032	1	2
C(5)	C	-0.1071(3)	0.70207(15)	0.99207(8)	0.029	1	2
C(4)	C	-0.4659(3)	0.58580(13)	0.90439(8)	0.025	1	2
C(3)	C	-0.3737(3)	0.44918(13)	0.87105(8)	0.025	1	2
C(1)	C	-0.0946(3)	0.35755(13)	0.78568(9)	0.028	1	2
C(2)	C	-0.4621(3)	0.42162(14)	0.73193(8)	0.028	1	2
C(8)	C	-0.1429(2)	0.62194(11)	0.79781(6)	0.017	1	2
C(7)	C	-0.1351(2)	0.73717(11)	0.85839(6)	0.017	1	2
C(12)	C	0.0062(2)	0.87160(12)	0.85678(7)	0.021	1	2
C(11)	C	0.1308(2)	0.90057(11)	0.79706(7)	0.021	1	2
C(10)	C	0.1063(2)	0.78940(11)	0.73320(6)	0.018	1	2
C(9)	C	-0.0265(2)	0.65300(11)	0.73570(7)	0.018	1	2
C(13)	C	0.2914(3)	1.04559(15)	0.80323(9)	0.032	1	2
C(14)	C	0.2187(2)	0.81461(11)	0.66418(7)	0.02	1	2
C(15)	C	0.3510(3)	0.72109(14)	0.63276(9)	0.034	1	2
C(16)	C	0.1747(2)	0.94385(11)	0.63020(6)	0.017	1	2
C(17)	C	-0.0283(2)	1.00290(12)	0.64011(7)	0.021	1	2
C(18)	C	-0.0648(2)	1.12673(12)	0.61021(7)	0.021	1	2
C(19)	C	0.1010(2)	1.19450(11)	0.56959(6)	0.018	1	2
C(20)	C	0.3040(2)	1.13625(12)	0.55888(7)	0.022	1	2
C(21)	C	0.3388(2)	1.01257(12)	0.58884(7)	0.02	1	2
C(22)	C	0.0593(3)	1.32786(12)	0.53956(7)	0.023	1	2
H(2)	H	0.184(4)	1.464(3)	0.4789(13)	0.076(8)	1	2
H(6A)	H	-0.484(3)	0.8767(17)	0.9052(10)	0.056(6)	1	2
H(6B)	H	-0.502(3)	0.8336(17)	0.9963(10)	0.059(5)	1	2
H(6C)	H	-0.261(3)	0.9562(19)	0.9690(9)	0.059(5)	1	2
H(5A)	H	0.029(3)	0.8003(17)	1.0099(9)	0.048(5)	1	2
H(5B)	H	-0.205(4)	0.6817(19)	1.0417(11)	0.073(6)	1	2
H(5C)	H	-0.010(3)	0.6122(18)	0.9804(10)	0.060(5)	1	2
H(4A)	H	-0.598(3)	0.6122(14)	0.8635(9)	0.044(4)	1	2
H(4B)	H	-0.560(3)	0.5652(14)	0.9534(9)	0.042(4)	1	2
H(3A)	H	-0.245(3)	0.4231(14)	0.9112(9)	0.041(4)	1	2
H(3B)	H	-0.511(3)	0.3489(16)	0.8633(8)	0.048(4)	1	2
H(1A)	H	-0.021(3)	0.3540(14)	0.7294(9)	0.039(4)	1	2
H(1B)	H	0.054(4)	0.3882(18)	0.8302(11)	0.064(6)	1	2
H(1C)	H	-0.177(3)	0.2475(17)	0.7885(9)	0.049(5)	1	2
H(2A)	H	-0.396(3)	0.4341(16)	0.6771(10)	0.056(5)	1	2
H(2B)	H	-0.547(3)	0.3076(18)	0.7272(9)	0.050(5)	1	2
H(2C)	H	-0.604(4)	0.4813(18)	0.7412(10)	0.062(5)	1	2
H(12)	H	0.026(3)	0.9617(15)	0.9050(8)	0.040(4)	1	2

H(9)	H	-0.039(2)	0.5676(14)	0.6856(8)	0.030(4)	1	2
H(13A)	H	0.445(3)	1.0372(16)	0.7777(10)	0.060(5)	1	2
H(13B)	H	0.218(4)	1.1209(19)	0.7747(11)	0.070(6)	1	2
H(13C)	H	0.337(3)	1.0974(17)	0.8612(11)	0.065(5)	1	2
H(15A)	H	0.426(3)	0.7328(15)	0.5814(9)	0.047(5)	1	2
H(15B)	H	0.384(3)	0.6317(18)	0.6601(10)	0.057(5)	1	2
H(17)	H	-0.157(3)	0.9555(14)	0.6729(8)	0.040(4)	1	2
H(18)	H	-0.227(3)	1.1705(15)	0.6196(8)	0.045(4)	1	2
H(20)	H	0.435(3)	1.1894(15)	0.5307(8)	0.041(4)	1	2
H(21)	H	0.500(3)	0.9767(15)	0.5816(9)	0.045(4)	1	2

Table S6. Anisotropic displacement parameters for 1a

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
O(1) 0.0375(7) 0.0296(4) 0.0425(6) 0.0188(4) 0.0169(5) 0.0234(4)
O(2) 0.0394(7) 0.0312(5) 0.0448(7) 0.0133(5) 0.0171(5) 0.0249(5)
C(01) 0.0225(8) 0.0124(5) 0.0213(6) -0.0001(5) 0.0028(6) 0.0049(4)
C(02) 0.0246(8) 0.0175(5) 0.0188(6) 0.0043(5) 0.0052(6) 0.0048(5)
C(6) 0.0376(10) 0.0253(7) 0.0364(9) 0.0123(6) 0.0114(8) 0.0037(6)
C(5) 0.0356(9) 0.0321(7) 0.0206(7) 0.0045(6) 0.0006(7) 0.0094(6)
C(4) 0.0247(8) 0.0238(6) 0.0260(7) 0.0002(5) 0.0084(7) 0.0055(5)
C(3) 0.0331(9) 0.0168(6) 0.0249(7) -0.0016(5) 0.0077(7) 0.0076(5)
C(1) 0.0312(9) 0.0157(6) 0.0400(9) 0.0055(5) 0.0081(8) 0.0073(6)
C(2) 0.0288(9) 0.0247(6) 0.0276(8) -0.0063(6) -0.0032(7) 0.0073(5)
C(8) 0.0205(7) 0.0118(5) 0.0173(6) 0.0003(5) 0.0030(5) 0.0037(4)
C(7) 0.0217(7) 0.0123(5) 0.0163(6) 0.0007(4) 0.0021(5) 0.0046(4)
C(12) 0.0297(8) 0.0137(5) 0.0189(7) -0.0019(5) 0.0029(6) 0.0043(5)
C(11) 0.0268(8) 0.0138(5) 0.0199(6) -0.0031(5) 0.0012(6) 0.0055(5)
C(10) 0.0219(7) 0.0142(5) 0.0183(6) 0.0001(5) 0.0026(5) 0.0071(4)
C(9) 0.0239(7) 0.0128(5) 0.0191(6) -0.0001(5) 0.0049(6) 0.0059(5)
C(13) 0.0428(10) 0.0195(6) 0.0282(8) -0.0129(6) -0.0001(7) 0.0074(6)
C(14) 0.0235(8) 0.0179(5) 0.0219(7) 0.0052(5) 0.0061(6) 0.0094(5)
C(15) 0.0453(10) 0.0272(7) 0.0407(9) 0.0196(6) 0.0238(8) 0.0196(6)
C(16) 0.0182(7) 0.0168(5) 0.0178(6) 0.0026(5) 0.0030(5) 0.0078(4)
C(17) 0.0194(8) 0.0214(6) 0.0256(7) 0.0040(5) 0.0063(6) 0.0121(5)
C(18) 0.0206(8) 0.0216(6) 0.0246(7) 0.0048(5) 0.0045(6) 0.0120(5)
C(19) 0.0226(8) 0.0161(5) 0.0182(6) 0.0038(5) 0.0033(6) 0.0085(4)
C(20) 0.0255(8) 0.0201(6) 0.0246(7) 0.0060(5) 0.0096(6) 0.0124(5)
C(21) 0.0217(8) 0.0197(6) 0.0241(7) 0.0052(5) 0.0083(6) 0.0119(5)
C(22) 0.0289(9) 0.0201(6) 0.0236(7) 0.0082(5) 0.0063(6) 0.0116(5)
```

Table S7. Multipole parameters for 1a

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
    _atom_rho_multipole_coeff_P1-1
```

```
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
O(1) 6.1166 0
0 0 -0.0675
0.0293 0 0 -0.1531 0
0.0283 0 0 0.0172 0 0 0
-0.0118 0 0 0.0113 0 0 0 -0.0026 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004


O(2) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


C(01) 3.9904 0
0 0 0.0002
0.0001 0 0 0 0
0.2157 0 0 0 0 0.1761 0
0.0438 0 0 0 0 -0.068 0 0 0
1.015965 1 1 1 1 1


C(02) 3.9904 0
0 0 0.0002
0.0001 0 0 0 0
0.2157 0 0 0 0 0.1761 0
0.0438 0 0 0 0 -0.068 0 0 0
1.015965 1 1 1 1 1
```

```
C(6) 4 0
0 0 -0.0103
-0.0146 0 0 0 0
0.2303 0 0 0 0 0.1851 0
0.0274 0 0 0 0 -0.0891 0 0 0
1.010691 1 1 1 1 1


C(5) 4 0
0 0 -0.0103
-0.0146 0 0 0 0
0.2303 0 0 0 0 0.1851 0
0.0274 0 0 0 0 -0.0891 0 0 0
1.010691 1 1 1 1 1


C(4) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1


C(3) 3.9428 0
0 0 0.0068
-0.0023 0 0 0.0044 0
-0.0061 0 0 -0.2812 0 0 0
-0.0696 0 0 0.0156 0 0 0 0.048 0
1.01237 1 1 1 1 1


C(1) 4 0
0 0 -0.0103
-0.0146 0 0 0 0
0.2303 0 0 0 0 0.1851 0
0.0274 0 0 0 0 -0.0891 0 0 0
1.010691 1 1 1 1 1


C(2) 4 0
0 0 -0.0103
-0.0146 0 0 0 0
0.2303 0 0 0 0 0.1851 0
0.0274 0 0 0 0 -0.0891 0 0 0
1.010691 1 1 1 1 1


C(8) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1
```

```
C(7) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1


C(12) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(11) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1


C(10) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1


C(9) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(13) 3.8152 0
0 0 0.0105
-0.0042 0 0 0 0
0.2189 0 0 0 0 0.1664 0
0.0291 0 0 0 0 -0.0668 0 0 0
1.018201 1 1 1 1 1


C(14) 4.0496 0
0 0 0.0529
0.1303 0 0 -0.1148 0
0.1668 0 0 0.1898 0 0 0
-0.0176 0 0 -0.0056 0 0 0 0.0142 0
1.016433 1 1 1 1 1


C(15) 3.9346 0
0 0 0.0644
```

```
0.1329 0 0 -0.118 0
0.1525 0 0 0.1882 0 0 0
-0.0159 0 0 -0.0135 0 0 0 0.0228 0
1.01604 1 1 1 1 1


C(16) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1


C(17) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(18) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(19) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1


C(20) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(21) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(22) 3.9888 0
0.0778 -0.0438 0
-0.2417 0 0 0.0853 0.0499
0 0.0167 -0.0152 0 0 0.3037 -0.0254
```

```
0.0143 0 0 0.0075 0.0018 0 0 -0.0649 0.019
1.015931 1 1 1 1 1


H(2) 0.9836 0
0.1799 0.0343 0
-0.0969 0 0 0.1745 -0.0122
0 -0.0337 -0.0181 0 0 0.0523 0.0583
0.0224 0 0 -0.0119 -0.0179 0 0 0.0025 0.0049
1.016284 1.2 1.2 1.2 1.2 1.2


H(6A) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(6B) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(6C) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(5A) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(5B) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(5C) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2
```

```
H(4A) 1.0212 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(4B) 1.0212 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(3A) 1.0212 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(3B) 1.0212 0
0 0 0.1444
0.0627 0 0 0 0
0.0158 0 0 0 0 0 0
-0.0004 0 0 0 0 0 0 0 0
1.127115 1.2 1.2 1.2 1.2 1.2


H(1A) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(1B) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(1C) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2
```

```
H(2A) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(2B) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(2C) 0.9808 0
0 0 0.1322
0.0462 0 0 0 0
0.0064 0 0 0 0 0 0
0.0008 0 0 0 0 0 0 0 0
1.138421 1.2 1.2 1.2 1.2 1.2


H(12) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(9) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(13A) 1.0212 0
0 0 0.1532
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(13B) 1.0212 0
0 0 0.1532
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(13C) 1.0212 0
0 0 0.1532
```

```
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(15A) 1.0135 0
0 0 0.1534
0.0613 0 0 0 0
0.0137 0 0 0 0 0 0
0.0044 0 0 0 0 0 0 0 0
1.12308 1.2 1.2 1.2 1.2 1.2


H(15B) 1.0135 0
0 0 0.1534
0.0613 0 0 0 0
0.0137 0 0 0 0 0 0
0.0044 0 0 0 0 0 0 0 0
1.12308 1.2 1.2 1.2 1.2 1.2


H(17) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(18) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(20) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(21) 0.9954 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

Tables S8 - S10 Disila-Bexarotene (1b)

Table S8. Atomic coordinates for 1b

```
loop_
    _atom_site_label
    _atom_site_type_symbol
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
```

Si(1)	Si	1.15990(5)	0.49708(2)	0.213229(19)	0.018	1	2
Si(2)	Si	1.25016(5)	0.31344(2)	0.375599(19)	0.021	1	2
O(1)	O	1.05821(15)	0.01957(7)	-0.37705(5)	0.034	1	2
O(2)	O	0.77230(17)	0.07361(7)	-0.46397(6)	0.037	1	2
C(1)	C	1.3445(2)	0.50600(9)	0.10937(8)	0.029	1	2
C(2)	C	0.9569(2)	0.59426(9)	0.20720(10)	0.031	1	2
C(3)	C	1.3321(2)	0.51880(9)	0.33902(8)	0.027	1	2
C(4)	C	1.4511(2)	0.42473(9)	0.36044(8)	0.027	1	2
C(5)	C	1.3976(3)	0.19790(12)	0.38817(13)	0.044	1	2
C(6)	C	1.1007(3)	0.34292(14)	0.49093(9)	0.043	1	2
C(7)	C	1.04117(18)	0.29067(7)	0.26030(7)	0.019	1	2
C(8)	C	1.00759(17)	0.36506(7)	0.19477(6)	0.017	1	2
C(9)	C	0.85210(18)	0.33911(7)	0.10923(7)	0.018	1	2
C(10)	C	0.72455(18)	0.24488(7)	0.08858(7)	0.017	1	2
C(11)	C	0.75169(19)	0.17243(7)	0.15582(7)	0.022	1	2
C(12)	C	0.9110(2)	0.19655(8)	0.23922(7)	0.023	1	2
C(13)	C	0.6126(3)	0.07111(9)	0.13954(10)	0.034	1	2
C(14)	C	0.56236(18)	0.22535(7)	-0.00439(7)	0.019	1	2
C(15)	C	0.3525(2)	0.24463(9)	0.00261(8)	0.029	1	2
C(16)	C	0.64216(18)	0.18514(7)	-0.10200(7)	0.018	1	2
C(17)	C	0.83101(19)	0.13261(8)	-0.10140(7)	0.022	1	2
C(18)	C	0.9091(2)	0.09346(8)	-0.19158(7)	0.024	1	2
C(19)	C	0.79946(19)	0.10556(8)	-0.28495(7)	0.022	1	2
C(20)	C	0.6100(2)	0.15742(8)	-0.28692(7)	0.025	1	2
C(21)	C	0.5335(2)	0.19691(8)	-0.19653(7)	0.024	1	2
C(22)	C	0.8885(2)	0.06297(8)	-0.37942(7)	0.025	1	2
H(2)	H	0.839(4)	0.0354(16)	-0.5243(17)	0.061(6)	1	2
H(1A)	H	1.478(3)	0.4597(12)	0.1198(11)	0.054(5)	1	2
H(1B)	H	1.408(3)	0.5812(13)	0.1102(11)	0.045(4)	1	2
H(1C)	H	1.257(3)	0.4764(13)	0.0391(14)	0.063(5)	1	2
H(2A)	H	1.045(4)	0.6677(16)	0.2202(14)	0.076(6)	1	2
H(2B)	H	0.851(4)	0.5923(14)	0.2636(14)	0.070(6)	1	2
H(2C)	H	0.867(3)	0.5874(13)	0.1341(14)	0.060(5)	1	2
H(3A)	H	1.457(3)	0.5900(15)	0.3399(12)	0.066(5)	1	2
H(3B)	H	1.231(3)	0.5408(13)	0.4016(13)	0.061(5)	1	2
H(4A)	H	1.563(3)	0.4419(13)	0.4326(13)	0.061(5)	1	2
H(4B)	H	1.548(3)	0.4011(13)	0.2940(13)	0.059(5)	1	2
H(5A)	H	1.520(4)	0.2132(18)	0.4434(18)	0.101(8)	1	2
H(5B)	H	1.460(4)	0.1767(18)	0.3237(18)	0.095(8)	1	2
H(5C)	H	1.286(5)	0.140(2)	0.4057(17)	0.108(9)	1	2
H(6A)	H	1.203(4)	0.3562(18)	0.5541(19)	0.101(8)	1	2
H(6B)	H	0.989(4)	0.2804(17)	0.4974(15)	0.085(7)	1	2
H(6C)	H	1.010(4)	0.4057(17)	0.4833(15)	0.084(7)	1	2
H(9)	H	0.823(2)	0.3936(10)	0.0567(10)	0.035(4)	1	2

H(12)	H	0.936(2)	0.1392(11)	0.2865(10)	0.040(4)	1	2
H(13A)	H	0.446(4)	0.0816(15)	0.1274(14)	0.076(6)	1	2
H(13B)	H	0.638(3)	0.0299(12)	0.2036(12)	0.053(4)	1	2
H(13C)	H	0.654(3)	0.0246(15)	0.0735(15)	0.077(6)	1	2
H(15A)	H	0.226(3)	0.2322(12)	-0.0626(12)	0.053(4)	1	2
H(15B)	H	0.295(3)	0.2743(13)	0.0758(13)	0.059(5)	1	2
H(17)	H	0.921(3)	0.1234(11)	-0.0296(11)	0.045(4)	1	2
H(18)	H	1.053(3)	0.0518(10)	-0.1909(10)	0.040(4)	1	2
H(20)	H	0.527(3)	0.1665(11)	-0.3596(11)	0.042(4)	1	2
H(21)	H	0.395(3)	0.2389(11)	-0.1971(10)	0.045(4)	1	2

Table S9. Anisotropic displacement parameters for 1b

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
Si(1) 0.01670(17) 0.01940(14) 0.01672(12) -0.00137(11) -0.00121(10) -
0.00039(10)
Si(2) 0.02070(19) 0.02753(15) 0.01430(13) 0.00152(12) -0.00219(10) 0.00203(10)
O(1) 0.0386(6) 0.0479(5) 0.0171(4) 0.0175(4) 0.0038(3) 0.0006(3)
O(2) 0.0464(6) 0.0490(5) 0.0176(4) 0.0192(5) 0.0010(3) 0.0010(3)
C(1) 0.0305(8) 0.0284(6) 0.0267(5) -0.0026(5) 0.0071(5) 0.0048(4)
C(2) 0.0267(8) 0.0254(6) 0.0384(6) 0.0039(5) -0.0022(5) -0.0019(5)
C(3) 0.0274(7) 0.0288(6) 0.0219(5) -0.0028(5) -0.0058(4) -0.0029(4)
C(4) 0.0221(7) 0.0354(6) 0.0221(5) -0.0021(5) -0.0057(4) 0.0018(4)
C(5) 0.0391(10) 0.0404(8) 0.0515(9) 0.0109(7) -0.0100(7) 0.0118(6)
C(6) 0.0413(10) 0.0655(10) 0.0200(6) -0.0042(8) 0.0066(5) -0.0022(6)
C(7) 0.0203(6) 0.0210(5) 0.0148(4) 0.0001(4) -0.0014(4) 0.0014(3)
C(8) 0.0174(6) 0.0198(5) 0.0129(4) -0.0008(4) -0.0013(3) 0.0003(3)
C(9) 0.0180(6) 0.0185(5) 0.0151(4) -0.0015(4) -0.0017(4) 0.0012(3)
C(10) 0.0175(6) 0.0190(5) 0.0143(4) -0.0004(4) -0.0005(3) -0.0011(3)
C(11) 0.0248(7) 0.0197(5) 0.0198(4) -0.0031(4) -0.0011(4) 0.0013(4)
C(12) 0.0276(7) 0.0214(5) 0.0188(4) -0.0012(4) -0.0034(4) 0.0052(4)
C(13) 0.0392(9) 0.0243(6) 0.0334(6) -0.0089(5) -0.0061(5) 0.0049(5)
C(14) 0.0164(6) 0.0210(5) 0.0169(4) -0.0001(4) -0.0002(4) -0.0026(3)
C(15) 0.0180(7) 0.0412(6) 0.0247(5) 0.0051(5) 0.0001(4) -0.0052(4)
C(16) 0.0183(6) 0.0199(5) 0.0152(4) 0.0001(4) -0.0007(4) -0.0015(3)
C(17) 0.0206(6) 0.0286(5) 0.0149(4) 0.0051(4) -0.0004(4) -0.0009(4)
C(18) 0.0240(7) 0.0306(5) 0.0170(5) 0.0066(5) 0.0007(4) -0.0007(4)
C(19) 0.0264(7) 0.0241(5) 0.0144(4) 0.0039(4) 0.0015(4) -0.0006(4)
C(20) 0.0294(7) 0.0302(5) 0.0158(4) 0.0070(5) -0.0008(4) 0.0009(4)
C(21) 0.0242(7) 0.0280(5) 0.0177(5) 0.0066(5) -0.0020(4) 0.0002(4)
C(22) 0.0331(7) 0.0258(5) 0.0159(4) 0.0070(5) 0.0036(4) -0.0002(4)
```

Table S10. Multipole parameters for 1b

```
loop_
    _atom_rho_multipole_atom_label
    _atom_rho_multipole_coeff_Pv
    _atom_rho_multipole_coeff_P00
    _atom_rho_multipole_coeff_P11
```

```
    _atom_rho_multipole_coeff_P1-1
    _atom_rho_multipole_coeff_P10
    _atom_rho_multipole_coeff_P20
    _atom_rho_multipole_coeff_P21
    _atom_rho_multipole_coeff_P2-1
    _atom_rho_multipole_coeff_P22
    _atom_rho_multipole_coeff_P2-2
    _atom_rho_multipole_coeff_P30
    _atom_rho_multipole_coeff_P31
    _atom_rho_multipole_coeff_P3-1
    _atom_rho_multipole_coeff_P32
    _atom_rho_multipole_coeff_P3-2
    _atom_rho_multipole_coeff_P33
    _atom_rho_multipole_coeff_P3-3
    _atom_rho_multipole_coeff_P40
    _atom_rho_multipole_coeff_P41
    _atom_rho_multipole_coeff_P4-1
    _atom_rho_multipole_coeff_P42
    _atom_rho_multipole_coeff_P4-2
    _atom_rho_multipole_coeff_P43
    _atom_rho_multipole_coeff_P4-3
    _atom_rho_multipole_coeff_P44
    _atom_rho_multipole_coeff_P4-4
    _atom_rho_multipole_kappa
    _atom_rho_multipole_kappa_prime0
    _atom_rho_multipole_kappa_prime1
    _atom_rho_multipole_kappa_prime2
    _atom_rho_multipole_kappa_prime3
    _atom_rho_multipole_kappa_prime4
Si(1) 3.8273 0
-0.0036 0.0028 0.0072
0.0007 -0.0055 -0.0059 0.003 0.0018
0.2865 -0.0018 -0.0002 -0.0065 -0.0031 0.0002 -0.2317
0.0587 0.0009 -0.0022 -0.0058 -0.0055 0.0016 0.0755 0.0028 0.0015
0.990386 1 1 1 1 1


Si(2) 3.8273 0
-0.0036 0.0028 0.0072
0.0007 -0.0055 -0.0059 0.003 0.0018
0.2865 -0.0018 -0.0002 -0.0065 -0.0031 0.0002 -0.2317
0.0587 0.0009 -0.0022 -0.0058 -0.0055 0.0016 0.0755 0.0028 0.0015
0.990386 1 1 1 1 1


O(1) 6.1166 0
0 0 -0.0675
0.0293 0 0 -0.1531 0
0.0283 0 0 0.0172 0 0 0
-0.0118 0 0 0.0113 0 0 0 -0.0026 0
1.003017 1.109004 1.109004 1.109004 1.109004 1.109004


O(2) 6.0788 0
-0.0536 -0.0866 0
0.1041 0 0 -0.028 0.042
0 -0.0147 -0.0263 0 0 0.065 -0.0215
0.0106 0 0 0.0042 0.0027 0 0 0.0149 0.0153
```

```
1.001632 1.113461 1.113461 1.113461 1.113461 1.113461


C(1) 3.7162 0
0 0 0.0172
0.0144 0 0 0 0
0.1648 0 0 0 0 0.1648 0
0.0127 0 0 0 0 -0.0579 0 0 0
1.017741 1 1 1 1 1


C(2) 3.7162 0
0 0 0.0172
0.0144 0 0 0 0
0.1648 0 0 0 0 0.1648 0
0.0127 0 0 0 0 -0.0579 0 0 0
1.017741 1 1 1 1 1


C(3) 4.2567 0
0.0333 -0.0382 0
0.0083 0 0 0.029 0.022
0 -0.1055 -0.203 0 0 0.1454 -0.0291
-0.0114 0 0 -0.0317 0.0769 0 0 0.0043 0.0161
1.001435 1 1 1 1 1


C(4) 4.2567 0
0.0333 -0.0382 0
0.0083 0 0 0.029 0.022
0 -0.1055 -0.203 0 0 0.1454 -0.0291
-0.0114 0 0 -0.0317 0.0769 0 0 0.0043 0.0161
1.001435 1 1 1 1 1


C(5) 3.7162 0
0 0 0.0172
0.0144 0 0 0 0
0.1648 0 0 0 0 0.1648 0
0.0127 0 0 0 0 -0.0579 0 0 0
1.017741 1 1 1 1 1


C(6) 3.7162 0
0 0 0.0172
0.0144 0 0 0 0
0.1648 0 0 0 0 0.1648 0
0.0127 0 0 0 0 -0.0579 0 0 0
1.017741 1 1 1 1 1


C(7) 4.1421 0
0.0238 -0.0021 0
-0.1791 0 0 0.005 -0.0026
0 0.0007 0.0034 0 0 0.2038 0.0243
0.0071 0 0 0.0032 0.0017 0 0 -0.0172 -0.0024
1.00633 1 1 1 1 1
```

C(8) 4.1421 0
0.0238 -0.0021 0
-0.1791 0 0 0.005 -0.0026
0 0.0007 0.0034 0 0 0.2038 0.0243
0.0071 0 0 0.0032 0.0017 0 0 -0.0172 -0.0024
1.00633 1 1 1 1 1

C(9) 3.9596 0
0.0166 0.0354 0
-0.1753 0 0 0.013 -0.0221
0 0.0108 0.022 0 0 0.2313 0.007
0.0164 0 0 0.008 -0.0146 0 0 0.0014 0
1.015464 1 1 1 1 1

C(10) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1

C(11) 4.0587 0
0.0178 0.0231 0
-0.1669 0 0 0.0156 -0.0213
0 0.0165 0.0239 0 0 0.231 -0.0068
0.0121 0 0 0.0076 -0.0048 0 0 0.0016 0
1.014932 1 1 1 1 1

C(12) 3.9596 0
0.0166 0.0354 0
-0.1753 0 0 0.013 -0.0221
0 0.0108 0.022 0 0 0.2313 0.007
0.0164 0 0 0.008 -0.0146 0 0 0.0014 0
1.015464 1 1 1 1 1

C(13) 3.8152 0
0 0 0.0105
-0.0042 0 0 0 0
0.2189 0 0 0 0 0.1664 0
0.0291 0 0 0 0 -0.0668 0 0 0
1.018201 1 1 1 1 1

C(14) 4.0496 0
0 0 0.0529
0.1303 0 0 -0.1148 0
0.1668 0 0 0.1898 0 0 0
-0.0176 0 0 -0.0056 0 0 0 0.0142 0
1.016433 1 1 1 1 1

C(15) 3.9346 0

```
0 0 0.0644
0.1329 0 0 -0.118 0
0.1525 0 0 0.1882 0 0 0
-0.0159 0 0 -0.0135 0 0 0 0.0228 0
1.01604 1 1 1 1 1


C(16) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1


C(17) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(18) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(19) 4.0553 0
0.0153 0.0288 0
-0.1768 0 0 0.0102 -0.0228
0 0.0129 0.0248 0 0 0.2306 -0.0085
0.011 0 0 0.0011 -0.0102 0 0 0.0008 0.0036
1.014566 1 1 1 1 1


C(20) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(21) 3.984 0
0.0192 0.034 0
-0.1645 0 0 0.0111 -0.0246
0 0.0129 0.0243 0 0 0.2299 0.0061
0.0181 0 0 0.0089 -0.0132 0 0 0.0019 -0.0008
1.018201 1 1 1 1 1


C(22) 3.9888 0
0.0778 -0.0438 0
-0.2417 0 0 0.0853 0.0499
```

```
0 0.0167 -0.0152 0 0 0.3037 -0.0254
0.0143 0 0 0.0075 0.0018 0 0 -0.0649 0.019
1.015931 1 1 1 1 1


H(2) 0.9922 0
0.1799 0.0343 0
-0.0969 0 0 0.1745 -0.0122
0 -0.0337 -0.0181 0 0 0.0523 0.0583
0.0224 0 0 -0.0119 -0.0179 0 0 0.0025 0.0049
1.016284 1.2 1.2 1.2 1.2 1.2


H(1A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(1B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(1C) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(2A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(2B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(2C) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
```

```
1.114183 1.2 1.2 1.2 1.2 1.2


H(3A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(3B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(4A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(4B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(5A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(5B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(5C) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2
```

```
H(6A) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(6B) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(6C) 1.0291 0
0 0 0.1563
0.0668 0 0 0 0
0.0189 0 0 0 0 0 0
0.0047 0 0 0 0 0 0 0 0
1.114183 1.2 1.2 1.2 1.2 1.2


H(9) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(12) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(13A) 1.0298 0
0 0 0.1532
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(13B) 1.0298 0
0 0 0.1532
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(13C) 1.0298 0
```

```
0 0 0.1532
0.0659 0 0 0 0
0.0196 0 0 0 0 0 0
0.0059 0 0 0 0 0 0 0 0
1.122183 1.2 1.2 1.2 1.2 1.2


H(15A) 1.0221 0
0 0 0.1534
0.0613 0 0 0 0
0.0137 0 0 0 0 0 0
0.0044 0 0 0 0 0 0 0 0
1.12308 1.2 1.2 1.2 1.2 1.2


H(15B) 1.0221 0
0 0 0.1534
0.0613 0 0 0 0
0.0137 0 0 0 0 0 0
0.0044 0 0 0 0 0 0 0 0
1.12308 1.2 1.2 1.2 1.2 1.2


H(17) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(18) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(20) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2


H(21) 1.004 0
0 0 0.1546
0.0629 0 0 0 0
0.0127 0 0 0 0 0 0
-0.002 0 0 0 0 0 0 0 0
1.13642 1.2 1.2 1.2 1.2 1.2
```

Dipole moments in Debye (D) (origin: center of mass)

(1a): μ_x = -0.1; μ_y = -6.6; μ_z = 5.7; μ_{total} = 8.7

(1b): μ_x = -1.9; μ_y = 1.8; μ_z = 8.6; μ_{total} = 9.0

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry