Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Accurate Single Crystal and Gas-Phase Molecular Structures of Acenaphthene: A Starting Point in the Search for the Longest C–C Bond

Supporting Information

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Table S1: Computed anharmonic and observed vibrational frequencies of Ace and root-mean-square deviations (all values in cm^{-1})

expt.	PBE0	B3LYP	B3PW91	B3LYP-D3	TPSSh	B2PLYP
	def2-TZVP					
			A_1			
	3087	3061	3073	3058	3063	3079
	3066	3043	3046	3042	3040	3062
	3074	3030	3006	3028	3032	3043
	2947	2941	2934	2938	2942	2909
	1628	1598	1614	1600	1595	1602
1601 [a]	1625	1597	1612	1600	1589	1598
	1458	1454	1454	1453	1454	1469
	1451	1436	1444	1434	1436	1443
1424 [a]	1425	1422	1419	1424	1422	1426
1366 [a]	1383	1365	1375	1364	1363	1374
1255 [a]	1260	1252	1252	1253	1247	1253
	1220	1220	1219	1218	1216	1223
1173 [a]	1178	1180	1175	1184	1175	1181
	1057	1048	1051	1047	1047	1051
	1015	996	1008	998	992	1000
938 [a]	954	923	943	921	927	934
	808	809	805	809	801	809
	648	638	643	639	636	638
541 [a]	548	548	547	548	541	547
410 [a]	418	419	417	421	414	417
			A_2			

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Table S1 – continued from the previous page

expt.	PBE0	B3LYP	B3PW91	B3LYP-D3	TPSSh	B2PLYP
	def2-TZVP					
	2939	2906	2922	2906	2911	2935
	1220	1213	1217	1210	1213	1224
	1022	1017	1018	1019	1008	1055
	1173	1199	1139	1203	1173	1406
	954	962	937	961	954	1025
	771	774	767	772	770	802
	679	704	665	713	700	884
	456	464	452	462	453	485
236 [b]	229	233	230	234	227	237
97 [b]	55	85	64	93	75	85
	B_1					
2920 [a]	2958	2926	2941	2925	2931	2953
	1153	1149	1151	1147	1141	1161
	1159	1224	1130	1239	1151	1290
	1004	1005	996	1009	1042	1079
	888	928	857	933	944	812
778 [a]	803	805	798	803	802	823
	787	781	777	774	769	1342
	564	576	559	577	572	605
	479	488	475	490	477	520
222 [b]	207	215	207	216	212	217
171 [b]	154	160	154	162	157	163
	B_2					
	3090	3061	3074	3058	3066	3083
3051 [a]	3060	3034	3040	3032	3051	3063
	3025	3005	3018	3010	3024	3052
	2948	2933	2937	2930	2933	2957
	1643	1611	1629	1614	1611	1618
1487 [a]	1521	1505	1511	1505	1500	1505
	1485	1474	1476	1474	1470	1479
	1425	1431	1429	1428	1431	1443
	1373	1357	1364	1358	1359	1369
1277 [a]	1283	1279	1277	1278	1277	1285
	1235	1225	1229	1226	1226	1236
1212 [a]	1216	1214	1214	1214	1210	1218
	1160	1158	1158	1159	1158	1164
	1100	1096	1095	1097	1090	1097
1015 [a]	1035	1023	1030	1022	1024	1026
	843	830	819	830	821	834
	660	650	658	653	658	663
	504	506	504	506	497	503
	448	453	447	444	447	444
	RMSD					
	20	11	14	11	11	15

[a] From Ref. [1] .
[b] From Ref. [2] .

Table S2: Crystallographic data for Ace measured at different temperatures.

Empirical formula		$C_{12}H_{10}$	
M_r		154.20	
T [K]	95.0(2)	200.0(1)	317.5(1)
Crystal system		Orthorhombic	
Space group		$Pmc2_1$	
a [Å]	13.8073(7)	13.8982(4)	14.0080(8)
b [Å]	8.2291(7)	8.2537(3)	8.2826(4)
c [Å]	7.0858(4)	7.1540(2)	7.2443(4)
V [$Å^3$]	805.10(9)	820.65(4)	840.51(8)
Z	4	4	4
μ [mm^{-1}]	0.072	0.070	0.069
ρ_{calcd} [$Mg \cdot m^{-3}$]	1.272	1.248	1.219
$F(000)$	328	328	328
θ_{max} [^{0}]	60.08	36.319	30.03
Index ranges h	$-33 \leq h \leq 33$	$-23 \leq h \leq 23$	$-19 \leq h \leq 19$
Index ranges k	$-20 \leq k \leq 20$	$-13 \leq k \leq 13$	$-11 \leq k \leq 11$
Index ranges l	$-17 \leq l \leq 17$	$-11 \leq l \leq 11$	$-10 \leq l \leq 10$
Reflexes collected	106572	34080	21327
Independent reflexes	12162	4070	2549
R_{int}	0.0391	0.0331	0.0337
data/restraints/parameters	12162/1/206	4070/1/205	2549/1/206
GoF on F^2	1.189	1.101	1.130
R_1/wR_2 [$I > 2\sigma(I)$]	0.0259/0.0456	0.0236/0.0482	0.0255/0.0588
R_{ind}(all data)/wR_2	0.0327/0.0475	0.0293/0.0505	0.0298/0.0611
ρ_{fin} (max/min) [$e \cdot Å^{-3}$]	0.19/–0.19	0.13/–0.12	0.12/–0.08
Flack parameter	–3(3)	-2(3)	–4(3)
CCDC number	1867649	1867648	1867647

Table S3: Selected bond lengths and angles of Ace at different temperatures. A/B: independent molecules in the unit cell.[a]

	95 K		200 K		317 K	
	A	B	A	B	A	B
r(C1–C2)	1.5640(4)	1.5621(5)	1.5625(10)	1.5594(13)	1.552(2)	1.5539(18)
r(C1–C3)	1.5138(3)	1.5127(3)	1.5116(7)	1.5115(9)	1.5081(15)	1.5076(11)
r(C3–C4)	1.3752(3)	1.3750(3)	1.3732(7)	1.3720(7)	1.3658(12)	1.3680(11)
r(C3–C8)	1.4100(2)	1.4096(3)	1.4090(6)	1.4084(6)	1.4043(10)	1.4053(9)
r(C4–C5)	1.4225(3)	1.4223(4)	1.4199(8)	1.4201(8)	1.4148(14)	1.4150(13)
r(C5–C6)	1.3820(3)	1.3823(4)	1.3798(9)	1.3795(9)	1.3703(16)	1.3739(14)
r(C6–C7)	1.4212(2)	1.4215(3)	1.4204(6)	1.4200(7)	1.4157(11)	1.4176(10)
r(C7–C8)	1.4072(4)	1.4069(4)	1.4028(9)	1.4059(9)	1.4006(14)	1.3993(14)
$\angle$(C1–C3–C4)	132.451(17)	132.45(2)	132.47(5)	132.52(5)	132.53(8)	132.49(7)
$\angle$(C1–C3–C8)	108.842(16)	108.842(19)	108.85(4)	108.71(5)	108.78(8)	108.77(6)
$\angle$(C2–C1–C3)	104.930(10)	104.955(11)	104.94(3)	105.02(3)	105.03(4)	105.03(4)
$\angle$(C3–C4–C5)	118.741(19)	118.74(2)	118.80(5)	118.75(5)	118.72(10)	118.85(9)
$\angle$(C3–C8–C3)	112.46(2)	112.40(3)	112.42(6)	112.54(6)	112.39(10)	112.40(9)
$\angle$(C3–C8–C7)	123.772(11)	123.797(13)	123.79(3)	123.73(3)	123.80(5)	123.80(4)
$\angle$(C4–C3–C8)	118.706(17)	118.70(2)	118.68(5)	118.76(5)	118.69(9)	118.74(8)
$\angle$(C4–C5–C6)	122.485(19)	122.52(2)	122.39(5)	122.50(6)	122.59(10)	122.27(9)
$\angle$(C5–C6–C7)	119.822(19)	119.76(2)	119.89(5)	119.84(6)	119.95(10)	120.16(9)
$\angle$(C6–C7–C8)	116.474(13)	116.483(15)	116.45(3)	116.42(4)	116.24(6)	116.19(6)
$\angle$(C6–C7–C6)	127.05(3)	127.03(3)	127.10(7)	127.17(7)	127.53(13)	127.62(11)
τ (C3–C1–C2–C3[1])	0.00(3)	-0.00(3)	-0.00(7)	0.00(7)	0.00(13)	0.00(12)
τ (C3–C4–C5–C6)	0.20(3)	-0.12(3)	0.25(8)	-0.21(7)	0.13(11)	-0.07(14)

[a] Bond lengths are given in Å and angles in degrees. See Fig. 3 (main text) for atom labeling.

Table S4: Conditions of GED/MS experiments

Parameter/Camera setting	LD	SD
Nozzle-to-film distance, mm	598	338
Primary electron beam current, μA	0.95	1.47
Accelerating voltage, kV	85	87
Temperature of effusion cell, K	338(5)	340(5)
Wavelength of electrons, Å	0.04045(5)	0.04005(5)
Exposure time, s	70	73
Residual gas pressure, Torr		
-in diffraction chamber	2.8×10^{-6}	2.1×10^{-6}
-in mass-spectrometric block	5.0×10^{-7}	5.0×10^{-7}
Ionization voltage, V	50	50
Recorded films, substance/standard	6/2	6/2
s-range/Δs, Å^{-1}	1.2–16.3/0.1	2.5–29.6/0.1
Inflection points for background[a]	2	2
Experimental weighted R-factor, %[b]	4.05	6.65
Experimental R-factor, %[c]	6.75	12.39

[a] For levelled intensities of Ace.
[b] Calculated for experimental $sM(s)$ of Ace as $\left[\sum_i^N \sum_j^M w_j \left(s_j M_i(s_j) - s_j M_{\mathrm{av}}(s_j)\right)^2 / N \sum_j^M w_j (s_j M_{\mathrm{av}}(s_j))^2\right]^{1/2} \times 100\%$, where $s_j M_i(s_j)$ is the experimental molecular intensity from set i in point s_j, $s_j M_{\mathrm{av}}(s_j)$ is the average molecular intensity curve in the point s_j, w_j is the weight of the averaged $sM(s)$ calculated from the respective standard deviation as $1/\sigma^2$, N is the number of data sets, M is the number of points in each set.
[c] Calculated with all $w_j = 1$.

Table S5: The most intense peaks in the mass-spectra of Ace in GED/MS experiments in comparison to NIST data. [3]

Ion	m/z	I, %		
		LD	SD	NIST
$[M]^+$	154	100	100	100
$[M - C_2H_4]^+$	126	5	5	5
$[C_6H_4]^+$	76	25	24	30
$[C_5H_3]^+$	63	13	13	12
$[C_4H_3]^+$	51	6	5	6

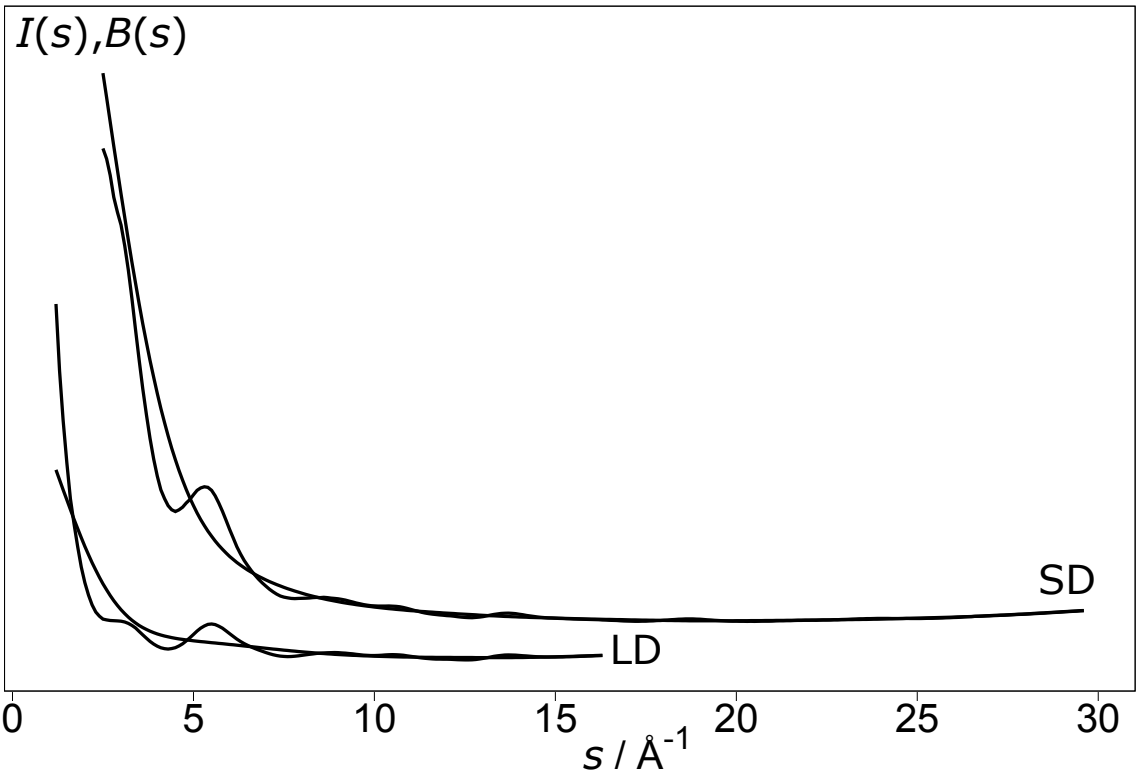

Figure S1: Total intensity functions measured for Ace and corresponding background lines. The data from the first diffraction patterns in LD and SD experiments are shown.

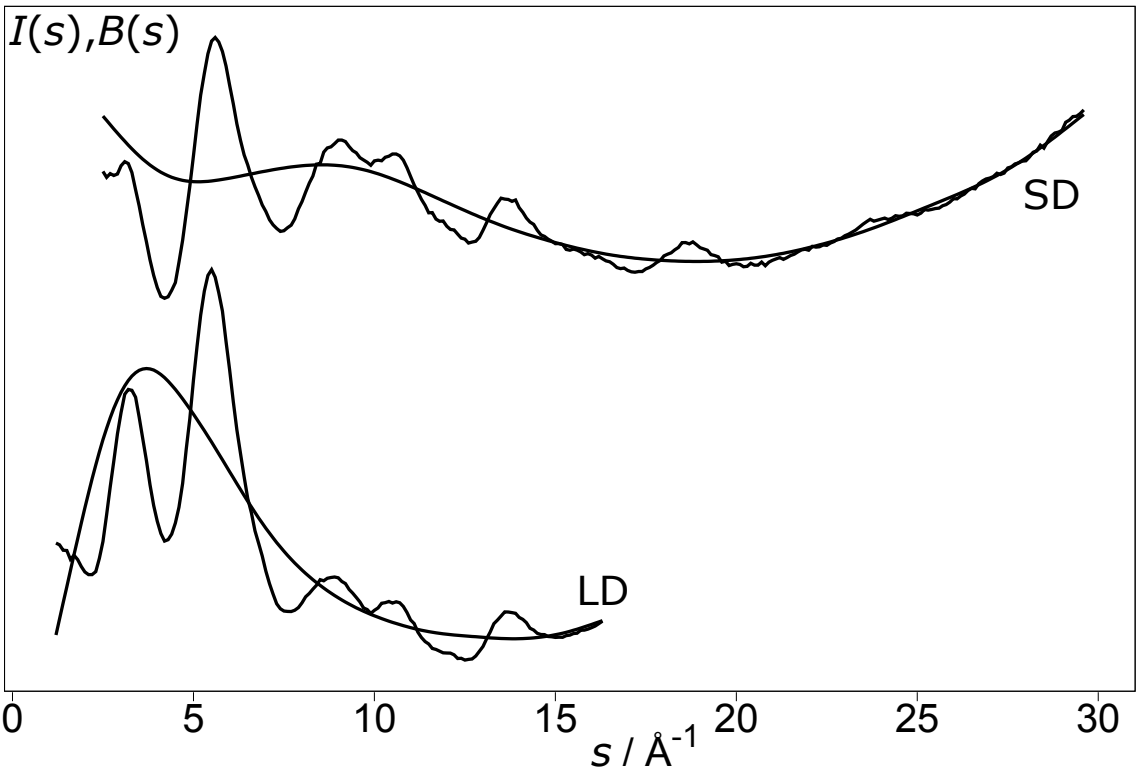

Figure S2: Levelled total intensity functions for Ace and corresponding background lines. The data from the first diffraction patterns in LD and SD experiments are shown.

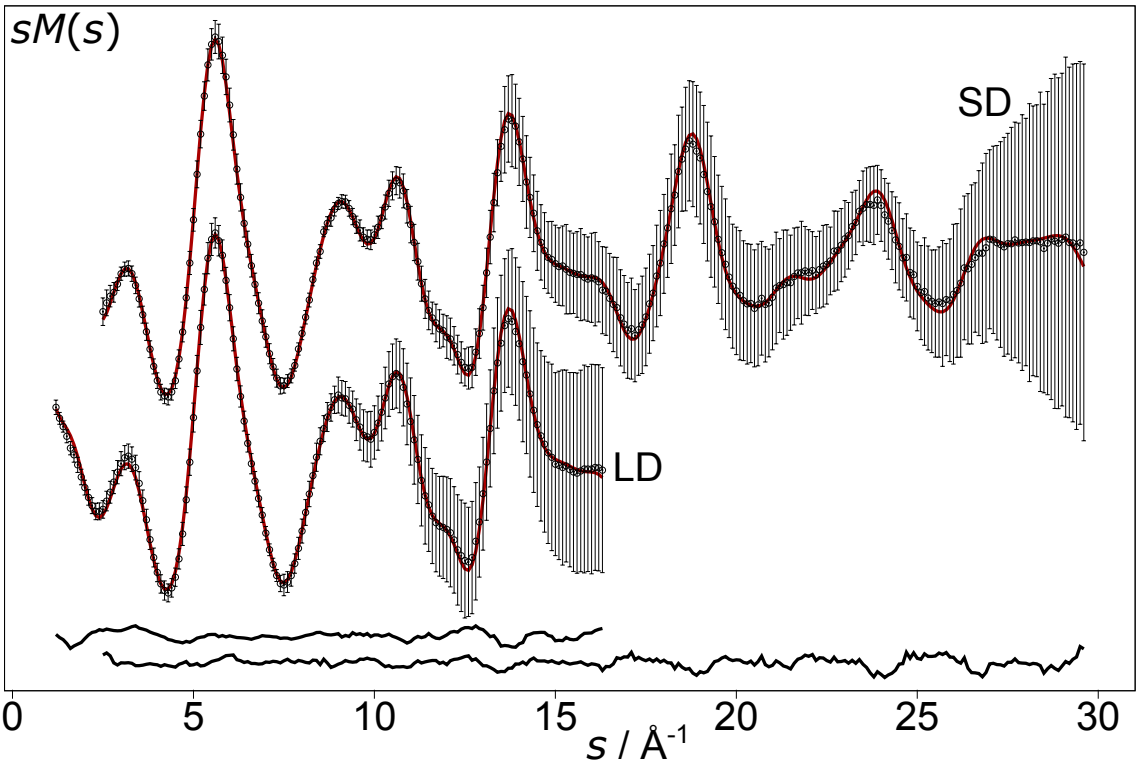

Figure S3: Molecular intensity functions for GED(II) refinement and corresponding difference curves.

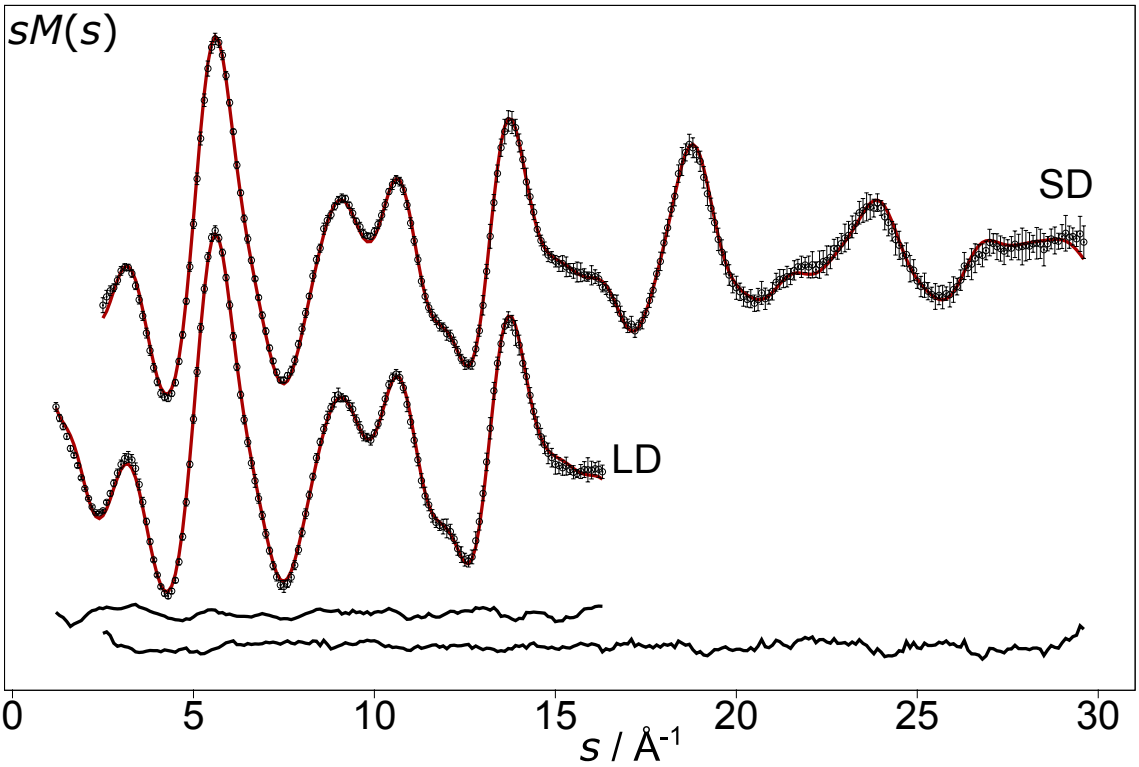

Figure S4: Molecular intensity functions for GED(III) refinement and corresponding difference curves.

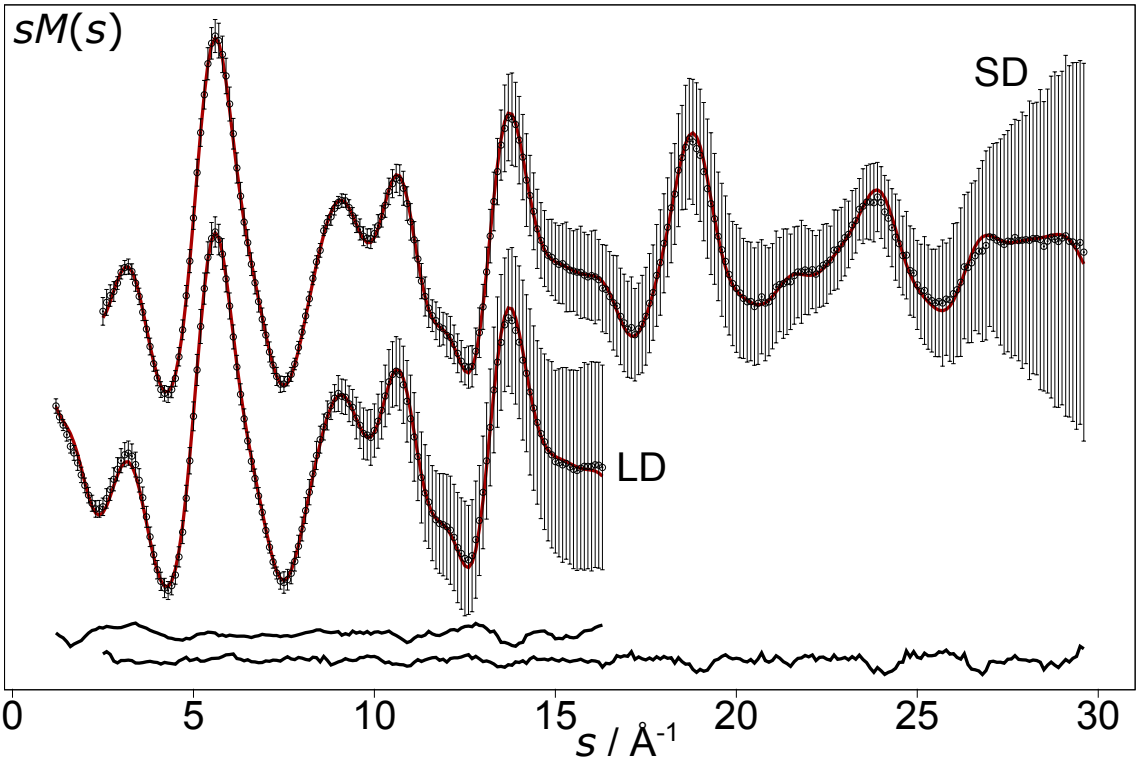

Figure S5: Molecular intensity functions for GED+MW(IV) refinement and corresponding difference curves.

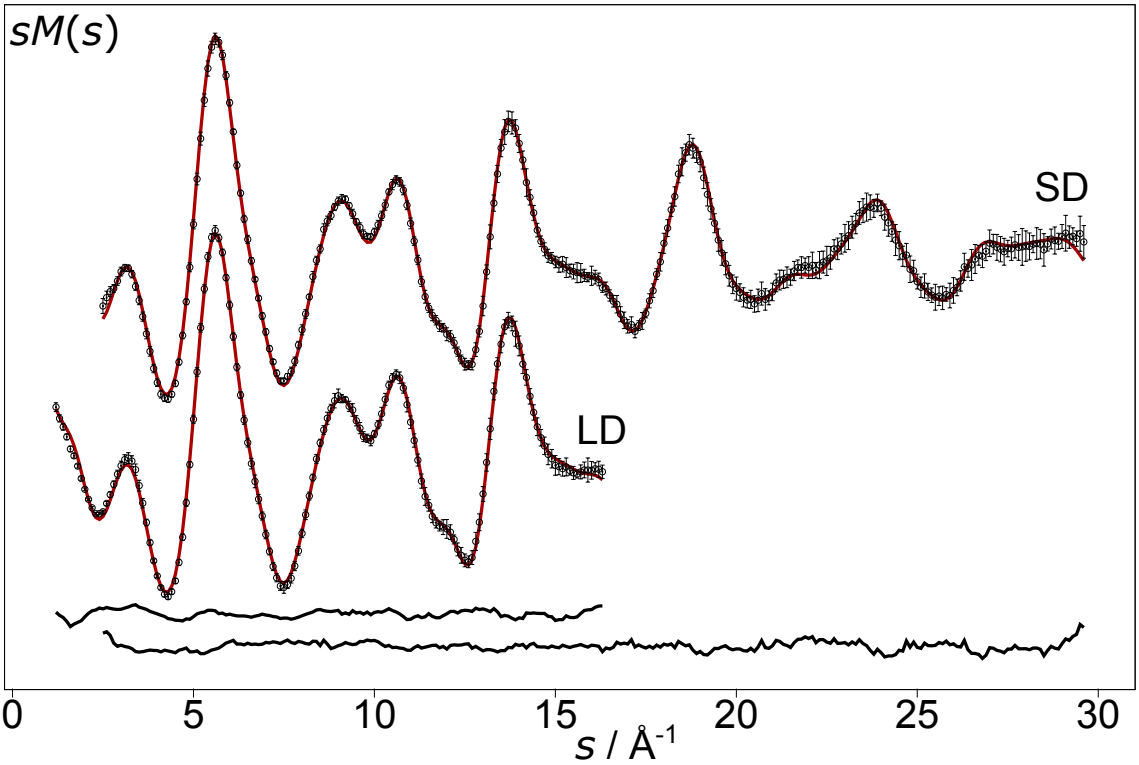

Figure S6: Molecular intensity functions for GED+MW(V) refinement and corresponding difference curves.

Table S6: Z-matrix used in the refinements of Ace.

1	C							
2	C	1	rCC1					
3	C	1	rCC2	2	aCCC1			
4	C	1	rCC2	2	aCCC1	3	180.	
5	C	3	rCC3	1	aCCC2	4	180.	
6	C	4	rCC3	1	aCCC2	3	180.	
7	C	5	rCC4	3	aCCC3	1	0.	
8	C	6	rCC4	4	aCCC3	1	0.	
9	C	7	rCC5	2	rCC6	1	180.	4
10	C	8	rCC5	2	rCC6	1	180.	4
11	X	1	rCX1	2	180.	9	90.	
12	C	11	rCX2	1	90.	3	0.	
13	C	11	rCX2	1	90.	4	0.	
14	H	5	rCH1	3	aHCC1	1	180.	
15	H	6	rCH1	4	aHCC1	1	180.	
16	H	7	rCH2	5	aHCC2	3	180.	
17	H	8	rCH2	6	aHCC2	4	180.	
18	H	9	rCH3	7	aHCC3	5	180.	
19	H	10	rCH3	8	aHCC3	6	180.	
20	H	12	rCH4	13	aHCC4	4	-dHCCC	
21	H	13	rCH4	12	aHCC4	3	-dHCCC	
22	H	12	rCH4	13	aHCC4	4	dHCCC	
23	H	13	rCH4	12	aHCC4	3	dHCCC	

rCC1	1.403870292382	1
rCC2	1.408896730400	2
rCC3	1.372676097002	3
rCC4	1.422114689932	4
rCC5	1.379295477837	5
rCC6	1.419643646537	6
rCX1	2.247569872508	7
rCX2	0.780882480886	8
rCH1	1.082660599864	9
rCH2	1.082454593784	10
rCH3	1.082782097640	11
rCH4	1.090781208376	12
aCCC1	123.786380877965	13
aCCC2	118.777148680451	14
aCCC3	118.681653187945	15
aHCC1	121.745482290821	16
aHCC2	118.579279033384	17
aHCC3	120.135713324778	18
aHCC4	111.330865904719	19
dHCCC	120.315092531532	20

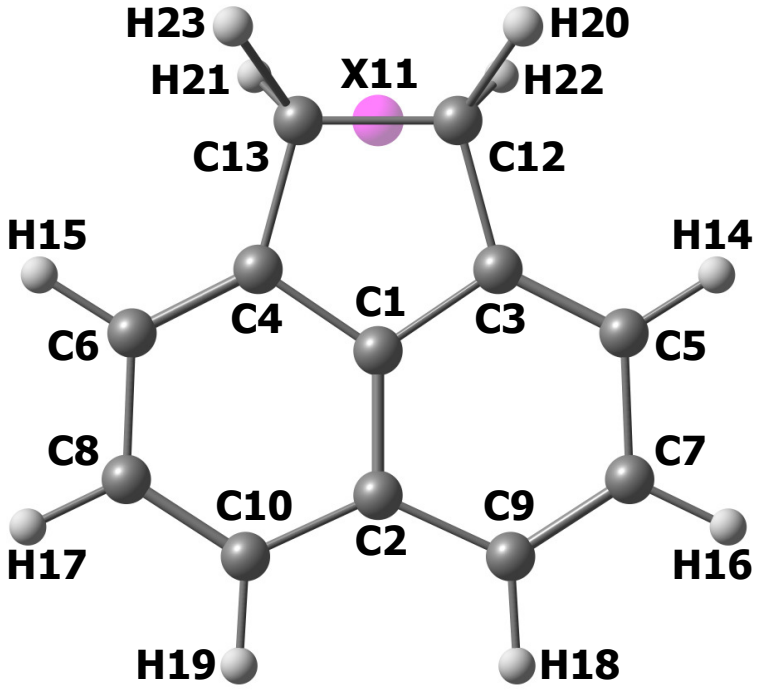

Figure S7: Geometrical model of Ace in refinements. Internal operational atom numbering is shown. X11 is the dummy atom in the center of the C12–C13 bond.

Table S7: Theoretical and experimental structural parameters of Ace from different variants of structural refinement. [a]

Method	CCSD(T)	MW [b] (I)	GED (II)	GED (III)	GED+MW (IV)	GED+MW (V)
r(C1–C2)	1.404	1.403(5)	1.403(5)	1.399(5)	1.402(4)	1.400(4)
r(C1–C3)	1.409	1.408(4)	1.408(4)	1.406(3)	1.407(4)	1.406(3)
r(C2–C9)	1.420	1.418(4)	1.419(5)	1.421(4)	1.418(4)	1.421(4)
r(C3–C5)	1.373	1.371(4)	1.371(5)	1.362(5)	1.370(4)	1.362(5)
r(C3–C12)	1.515	1.510(7)	1.515(8)	1.513(4)	1.512(6)	1.515(3)
r(C5–C7)	1.422	1.421(5)	1.423(5)	1.429(4)	1.423(5)	1.430(4)
r(C5–H14)	1.083	1.083(5)	1.083(5)	1.078(5)	1.082(5)	1.078(5)
r(C7–C9)	1.379	1.378(5)	1.380(5)	1.378(5)	1.379(5)	1.378(5)
r(C7–H16)	1.083	1.082(5)	1.083(5)	1.081(5)	1.082(5)	1.081(5)
r(C8–C10)	1.379	1.378(5)	1.380(5)	1.378(5)	1.379(5)	1.378(5)
r(C9–H18)	1.083	1.083(5)	1.083(5)	1.078(5)	1.082(5)	1.079(5)
r(C12–C13)	1.562	1.562(5)	1.563(5)	1.561(4)	1.563(5)	1.560(4)
r(C12–H20)	1.091	1.091(4)	1.091(5)	1.087(4)	1.091(4)	1.092(4)
WRMSD[c] bonds		0.002	0.001	0.005	0.002	0.004
∠(C2–C1–C3)	123.8	124.0(3)	123.9(3)	124.1(2)	124.0(2)	124.0(2)
∠(C1–C2–C9)	116.4	116.3(3)	116.1(9)	115.6(3)	116.2(3)	116.1(2)
∠(C3–C1–C4)	112.4	112.1(6)	112.3(7)	111.9(4)	112.1(5)	112.1(4)
∠(C1–C3–C5)	118.8	118.7(3)	118.9(4)	119.3(3)	118.8(3)	119.1(2)
∠(C1–C3–C12)	108.9	109.1(4)	109.0(5)	109.4(3)	109.2(4)	109.2(3)
∠(C9–C2–C10)	127.2	127.5(6)	127.7(18)	128.7(7)	127.5(6)	127.9(5)
∠(C2–C9–C7)	120.0	120.0(5)	120.3(13)	120.8(5)	120.0(4)	120.3(4)
∠(C2–C9–H18)	119.9	119.9(7)	119.5(14)	118.7(7)	119.8(7)	119.2(6)
∠(C5–C3–C12)	132.4	132.2(4)	132.1(6)	131.3(4)	132.0(4)	131.7(4)
∠(C3–C5–C7)	118.7	118.6(4)	118.7(4)	118.6(3)	118.6(4)	118.7(3)
∠(C3–C5–H14)	121.8	121.7(5)	121.7(5)	121.7(5)	121.7(5)	121.7(5)
∠(C3–C12–C13)	104.9	104.8(2)	104.8(2)	104.7(2)	104.8(2)	104.8(2)
∠(C3–C12–H20)	111.1	111.1(5)	111.2(5)	111.7(5)	111.1(5)	111.5(5)
∠(C7–C5–H14)	119.6	119.6(6)	119.6(7)	119.7(6)	119.7(6)	119.6(6)
∠(C5–C7–C9)	122.4	122.5(6)	122.1(10)	121.6(3)	122.4(5)	121.9(3)
∠(C5–C7–H16)	118.6	118.6(5)	118.6(5)	118.6(5)	118.6(5)	118.6(5)
∠(C9–C7–H16)	119.0	118.9(7)	119.3(11)	119.8(6)	119.0(7)	119.5(6)
∠(C7–C9–H18)	120.1	120.1(5)	120.2(5)	120.5(5)	120.2(5)	120.5(5)
∠(C13–C12–H20)	111.3	111.3(5)	111.4(5)	111.8(5)	111.3(5)	111.3(4)
∠(H20–C12–H22)	107.1	107.2(7)	106.8(9)	105.2(9)	107.2(7)	106.5(7)
WRMSD[c] angles		0.1	0.2	0.7	0.2	0.4
τ (C3–C12–C13–H23)	120.3	120.2(4)	120.4(5)	121.1(5)	120.2(4)	120.7(4)

[a] Bond lengths (Å) and angles (degrees) correspond to equilibrium structure. See Fig. S7 for atom numbering. [b] Numbers given in parentheses are 1 standard deviations from Monte-Carlo simulations. [c] Weighted root-mean-square deviations of refined parameters from CCSD(T) values.

Table S8: Contributions of MW and GED data into refined molecular parameters of Ace.[a]

Method	MW(I)	GED(II)	GED(III)	GED+MW(IV		GED+MW(V	
Parameter	w_{ROT}	w_{GED}	w_{GED}	w_{GED}	w_{ROT}	w_{GED}	w_{ROT}
r(C1–C2)	1.00	0.27	0.83	0.00	1.00	0.01	0.99
r(C1–C3)	1.00	0.53	0.91	0.00	1.00	0.01	0.99
r(C2–C9)	1.00	0.46	0.92	0.00	1.00	0.00	1.00
r(C3–C5)	1.00	0.45	0.91	0.00	1.00	0.01	0.99
r(C3–C12)	1.00	0.46	0.89	0.00	1.00	0.00	0.99
r(C5–C7)	1.00	0.46	0.91	0.00	1.00	0.01	0.99
r(C5–H14)	0.90	0.03	0.24	0.00	0.90	0.03	0.87
r(C7–C9)	1.00	0.47	0.92	0.00	1.00	0.01	0.99
r(C7–H16)	0.92	0.03	0.24	0.00	0.92	0.03	0.89
r(C8–C10)	1.00	0.47	0.92	0.00	1.00	0.01	0.99
r(C9–H18)	0.92	0.03	0.25	0.00	0.92	0.03	0.90
r(C12–C13)	1.00	0.28	0.75	0.00	1.00	0.01	0.99
r(C12–H20)	0.96	0.09	0.52	0.00	0.96	0.04	0.92
$\angle$(C2–C1–C3)	0.99	0.08	0.61	0.00	0.99	0.02	0.97
$\angle$(C1–C2–C9)	1.00	0.29	0.85	0.00	1.00	0.01	0.99
$\angle$(C3–C1–C4)	0.99	0.08	0.61	0.00	0.99	0.02	0.97
$\angle$(C1–C3–C5)	1.00	0.12	0.47	0.00	1.00	0.00	1.00
$\angle$(C1–C3–C12)	1.00	0.14	0.63	0.00	1.00	0.00	1.00
$\angle$(C9–C2–C10)	1.00	0.29	0.85	0.00	1.00	0.01	0.99
$\angle$(C2–C9–C7)	1.00	0.10	0.65	0.00	1.00	0.00	1.00
$\angle$(C2–C9–H18)	1.00	0.04	0.37	0.00	1.00	0.00	0.99
$\angle$(C2–C10–C8)	1.00	0.10	0.65	0.00	1.00	0.00	1.00
$\angle$(C5–C3–C12)	1.00	0.17	0.71	0.00	1.00	0.00	0.99
$\angle$(C3–C5–C7)	1.00	0.13	0.61	0.00	1.00	0.00	0.99
$\angle$(C3–C5–H14)	0.99	0.05	0.33	0.00	0.99	0.00	0.99
$\angle$(C3–C12–C13)	1.00	0.26	0.81	0.00	1.00	0.01	0.99
$\angle$(C3–C12–H20)	1.00	0.19	0.75	0.00	1.00	0.01	0.99
$\angle$(C7–C5–H14)	0.99	0.06	0.41	0.00	0.99	0.01	0.99
$\angle$(C5–C7–C9)	1.00	0.27	0.77	0.00	1.00	0.01	0.99
$\angle$(C5–C7–H16)	0.98	0.06	0.37	0.00	0.98	0.01	0.97
$\angle$(C9–C7–H16)	1.00	0.10	0.54	0.00	1.00	0.00	0.99
$\angle$(C7–C9–H18)	0.99	0.02	0.22	0.00	0.99	0.00	0.99
$\angle$(C13–C12–H20)	0.99	0.16	0.67	0.00	0.99	0.01	0.98
$\angle$(H20–C12–H22)	0.99	0.11	0.57	0.00	0.99	0.01	0.99
τ (C3–C12–C13–H23)	0.99	0.09	0.47	0.00	0.99	0.01	0.98

[a] The values calculated using the method described in Ref. [4] See Fig. S7 for atom numbering.

Table S9: Molecular parameters of naphthalene core of Ace and unsubstituted naphthalene optimized at r^{2}SCAN-3c level of theory.[a]

Parameter	Ace	naphthalene
r(C3–C4)	1.374	1.373
r(C3–C8)	1.406	1.416
r(C4–C5)	1.418	1.412
r(C5–C6)	1.380	1.373
r(C6–C7)	1.417	1.416
r(C7–C8)	1.411	1.431
∠(C3–C4–C5)	118.7	120.3
∠(C3–C8–C7)	123.7	118.9
∠(C4–C3–C8)	118.8	120.8
∠(C4–C5–C6)	122.5	120.3
∠(C5–C6–C7)	120.0	120.8
∠(C6–C7–C8)	116.3	118.9
∠(C3–C8–C3^1)	112.6	122.2
∠(C6–C7–C6^1)	127.4	122.2
d(C6...C6^1)	2.541	2.479
	2.553[b]	-
	2.545[c]	2.475 [d]

[a] Bond lengths (Å) and angles (degrees) correspond to equilibrium structure. [b] From GED+MW(V) refinement (this work). [c] From SC-XRD analysis at 95 K (this work). [d] From XRD study at 100 K.[5]

Table S10: GED terms (in Å) for the GED(II) refinement.

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	H16	1.098019	0.075600	0.075612	3.6e-03	-0.015500	100
C8	H17	1.098019	0.075600	0.075612	3.6e-03	-0.015500	100
C5	H14	1.098016	0.075700	0.075712	3.6e-03	-0.015400	100
C6	H15	1.098016	0.075700	0.075712	3.6e-03	-0.015400	100
C9	H18	1.098086	0.075600	0.075612	3.6e-03	-0.015500	100
C10	H19	1.098086	0.075600	0.075612	3.6e-03	-0.015500	100
C12	H20	1.107435	0.077100	0.077113	3.7e-03	-0.016800	100
C12	H22	1.107435	0.077100	0.077113	3.7e-03	-0.016800	100
C13	H21	1.107435	0.077100	0.077113	3.7e-03	-0.016800	100
C13	H23	1.107435	0.077100	0.077113	3.7e-03	-0.016800	100
C4	C6	1.376714	0.044100	0.044889	2.0e-03	-0.005600	101
C3	C5	1.376714	0.044100	0.044889	2.0e-03	-0.005600	101
C7	C9	1.387403	0.044600	0.045398	2.0e-03	-0.007700	101
C8	C10	1.387403	0.044600	0.045398	2.0e-03	-0.007700	101
C1	C3	1.414874	0.045700	0.046517	2.1e-03	-0.007150	101
C1	C4	1.414874	0.045700	0.046517	2.1e-03	-0.007150	101
C1	C2	1.406977	0.045500	0.046314	2.1e-03	-0.003700	101
C2	C10	1.426838	0.046600	0.047434	2.1e-03	-0.007500	101
C2	C9	1.426838	0.046600	0.047434	2.1e-03	-0.007500	101
C5	C7	1.431461	0.047100	0.047942	2.1e-03	-0.008200	101
C6	C8	1.431461	0.047100	0.047942	2.1e-03	-0.008200	101
C4	C13	1.521428	0.050900	0.051810	2.3e-03	-0.006500	101
C3	C12	1.521428	0.050900	0.051810	2.3e-03	-0.006500	101
C12	C13	1.566278	0.053700	0.054661	2.4e-03	-0.003400	101
H23	H21	1.773802	0.123600	0.124055	5.6e-03	-0.022300	102
H22	H20	1.773802	0.123600	0.124055	5.6e-03	-0.022300	102
C9	H16	2.144555	0.097600	0.097959	4.4e-03	-0.014000	102
C10	H17	2.144555	0.097600	0.097959	4.4e-03	-0.014000	102
C8	H19	2.153219	0.097600	0.097959	4.4e-03	-0.013600	102
C7	H18	2.153219	0.097600	0.097959	4.4e-03	-0.013600	102
C3	H14	2.160298	0.096700	0.097056	4.4e-03	-0.012300	102
C4	H15	2.160298	0.096700	0.097056	4.4e-03	-0.012300	102
C5	H16	2.175550	0.098900	0.099264	4.5e-03	-0.014200	102
C6	H17	2.175550	0.098900	0.099264	4.5e-03	-0.014200	102
C3	H20	2.178135	0.111000	0.111408	5.0e-03	-0.014500	102
C3	H22	2.178135	0.111000	0.111408	5.0e-03	-0.014500	102
C4	H23	2.178135	0.111000	0.111408	5.0e-03	-0.014500	102
C4	H21	2.178135	0.111000	0.111408	5.0e-03	-0.014500	102
C2	H19	2.181372	0.098500	0.098862	4.4e-03	-0.013800	102
C2	H18	2.181372	0.098500	0.098862	4.4e-03	-0.013800	102
C7	H14	2.186789	0.099000	0.099364	4.5e-03	-0.014600	102
C8	H15	2.186789	0.099000	0.099364	4.5e-03	-0.014600	102
C13	H22	2.218879	0.109700	0.110104	4.9e-03	-0.010700	102
C13	H20	2.218879	0.109700	0.110104	4.9e-03	-0.010700	102
C12	H23	2.218879	0.109700	0.110104	4.9e-03	-0.010700	102
C12	H21	2.218879	0.109700	0.110104	4.9e-03	-0.010700	102
C3	C4	2.347004	0.052900	0.053928	2.4e-03	-0.008800	103

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Table S10 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
H22	H21	2.395533	0.178500	0.179157	8.0e-03	-0.036700	102
H20	H23	2.395533	0.178500	0.179157	8.0e-03	-0.036700	102
C1	C12	2.381848	0.055300	0.056375	2.5e-03	-0.001300	103
C1	C13	2.381848	0.055300	0.056375	2.5e-03	-0.001300	103
C1	C6	2.403145	0.053600	0.054642	2.4e-03	-0.009800	103
C1	C5	2.403145	0.053600	0.054642	2.4e-03	-0.009800	103
C1	C9	2.403008	0.054900	0.055967	2.5e-03	-0.007600	103
C1	C10	2.403008	0.054900	0.055967	2.5e-03	-0.007600	103
C3	C7	2.412263	0.054800	0.055865	2.5e-03	-0.008250	103
C4	C8	2.412263	0.054800	0.055865	2.5e-03	-0.008250	103
C2	C8	2.438719	0.054400	0.055458	2.4e-03	-0.010500	103
C2	C7	2.438719	0.054400	0.055458	2.4e-03	-0.010500	103
C3	C13	2.436675	0.058300	0.059433	2.6e-03	0.002450	103
C4	C12	2.436675	0.058300	0.059433	2.6e-03	0.002450	103
H16	H18	2.467219	0.158100	0.158682	7.1e-03	-0.012550	102
H19	H17	2.467219	0.158100	0.158682	7.1e-03	-0.012550	102
C6	C10	2.463968	0.054700	0.055763	2.5e-03	-0.011400	103
C5	C9	2.463968	0.054700	0.055763	2.5e-03	-0.011400	103
H14	H16	2.489494	0.159300	0.159886	7.2e-03	-0.014200	102
H17	H15	2.489494	0.159300	0.159886	7.2e-03	-0.014200	102
C2	C4	2.488148	0.055400	0.056477	2.5e-03	-0.007900	103
C2	C3	2.488148	0.055400	0.056477	2.5e-03	-0.007900	103
C9	C10	2.559882	0.059600	0.060759	2.7e-03	-0.011300	103
C5	C12	2.650008	0.062800	0.064021	2.8e-03	-0.012200	103
C6	C13	2.650008	0.062800	0.064021	2.8e-03	-0.012200	103
H18	H19	2.688660	0.185300	0.185982	8.3e-03	-0.013900	102
C1	C7	2.744356	0.059500	0.060657	2.7e-03	-0.009300	103
C1	C8	2.744356	0.059500	0.060657	2.7e-03	-0.009300	103
C3	C9	2.823504	0.060800	0.061982	2.7e-03	-0.009050	103
C4	C10	2.823504	0.060800	0.061982	2.7e-03	-0.009050	103
C10	H18	2.839953	0.128500	0.128973	5.8e-03	-0.013500	102
C9	H19	2.839953	0.128500	0.128973	5.8e-03	-0.013500	102
C2	C6	2.863741	0.060900	0.062084	2.7e-03	-0.011200	103
C2	C5	2.863741	0.060900	0.062084	2.7e-03	-0.011200	103
H20	H21	2.942801	0.167200	0.167815	7.5e-03	-0.004800	102
H22	H23	2.942801	0.167200	0.167815	7.5e-03	-0.004800	102
C13	H15	2.980810	0.129400	0.129876	5.8e-03	-0.018200	102
C12	H14	2.980810	0.129400	0.129876	5.8e-03	-0.018200	102
C5	H20	3.026463	0.137400	0.137906	6.2e-03	-0.023300	102
C5	H22	3.026464	0.137400	0.137906	6.2e-03	-0.023300	102
C6	H21	3.026463	0.137400	0.137906	6.2e-03	-0.023300	102
C6	H23	3.026464	0.137400	0.137906	6.2e-03	-0.023300	102
H14	H20	3.116025	0.219600	0.220408	9.9e-03	-0.029600	102
H15	H21	3.116025	0.219600	0.220408	9.9e-03	-0.029600	102
H15	H23	3.116025	0.219600	0.220408	9.9e-03	-0.029600	102
H14	H22	3.116025	0.219600	0.220408	9.9e-03	-0.029600	102
C1	H21	3.120535	0.169750	0.170375	7.6e-03	0.008350	102
C1	H22	3.120535	0.169750	0.170375	7.6e-03	0.008350	102
C1	H20	3.120535	0.169750	0.170375	7.6e-03	0.008350	102

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Table S10 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C1	H23	3.120535	0.169750	0.170375	7.6e-03	0.008350	102
C4	H20	3.175235	0.184800	0.185480	8.3e-03	0.018000	102
C3	H21	3.175235	0.184800	0.185480	8.3e-03	0.018000	102
C4	H22	3.175235	0.184800	0.185480	8.3e-03	0.018000	102
C3	H23	3.175235	0.184800	0.185480	8.3e-03	0.018000	102
C4	H17	3.390033	0.094200	0.094547	4.2e-03	-0.014600	102
C3	H16	3.390033	0.094200	0.094547	4.2e-03	-0.014600	102
C1	H14	3.408155	0.092900	0.093242	4.2e-03	-0.016050	102
C1	H15	3.408155	0.092900	0.093242	4.2e-03	-0.016050	102
C1	H18	3.397924	0.093700	0.094045	4.2e-03	-0.013400	102
C1	H19	3.397924	0.093700	0.094045	4.2e-03	-0.013400	102
C2	H17	3.423522	0.094100	0.094446	4.2e-03	-0.017000	102
C2	H16	3.423522	0.094100	0.094446	4.2e-03	-0.017000	102
C10	H15	3.437005	0.095000	0.095350	4.3e-03	-0.017600	102
C9	H14	3.437005	0.095000	0.095350	4.3e-03	-0.017600	102
C5	H18	3.448158	0.094600	0.094948	4.3e-03	-0.017500	102
C6	H19	3.448158	0.094600	0.094948	4.3e-03	-0.017500	102
C3	C6	3.622830	0.057900	0.059026	2.6e-03	-0.010600	103
C4	C5	3.622830	0.057900	0.059026	2.6e-03	-0.010600	103
C3	C10	3.736922	0.060000	0.061166	2.7e-03	-0.011300	103
C4	C9	3.736922	0.060000	0.061166	2.7e-03	-0.011300	103
C2	C13	3.736184	0.060900	0.062084	2.7e-03	-0.001600	103
C2	C12	3.736184	0.060900	0.062084	2.7e-03	-0.001600	103
C8	C9	3.790255	0.062700	0.063919	2.8e-03	-0.013900	103
C7	C10	3.790255	0.062700	0.063919	2.8e-03	-0.013900	103
C5	C13	3.793362	0.064600	0.065856	2.9e-03	0.004400	103
C6	C12	3.793362	0.064600	0.065856	2.9e-03	0.004400	103
C1	H17	3.833300	0.092400	0.092740	4.2e-03	-0.015750	102
C1	H16	3.833300	0.092400	0.092740	4.2e-03	-0.015750	102
C8	C13	3.891634	0.066000	0.067283	3.0e-03	-0.011850	103
C7	C12	3.891634	0.066000	0.067283	3.0e-03	-0.011850	103
C3	H18	3.912020	0.093300	0.093643	4.2e-03	-0.015150	102
C4	H19	3.912020	0.093300	0.093643	4.2e-03	-0.015150	102
C2	H14	3.951816	0.093400	0.093744	4.2e-03	-0.017200	102
C2	H15	3.951816	0.093400	0.093744	4.2e-03	-0.017200	102
C3	C8	4.148909	0.062900	0.064123	2.8e-03	-0.011700	103
C4	C7	4.148909	0.062900	0.064123	2.8e-03	-0.011700	103
C8	H18	4.205069	0.128000	0.128471	5.8e-03	-0.016150	102
C7	H19	4.205069	0.128000	0.128471	5.8e-03	-0.016150	102
C6	C9	4.278862	0.065100	0.066366	2.9e-03	-0.014100	103
C5	C10	4.278862	0.065100	0.066366	2.9e-03	-0.014100	103
H19	H15	4.326900	0.130600	0.131081	5.9e-03	-0.021600	102
H14	H18	4.326900	0.130600	0.131081	5.9e-03	-0.021600	102
C7	H22	4.324027	0.142100	0.142623	6.4e-03	-0.017350	102
C8	H23	4.324027	0.142100	0.142623	6.4e-03	-0.017350	102
C8	H21	4.324027	0.142100	0.142623	6.4e-03	-0.017350	102
C7	H20	4.324027	0.142100	0.142623	6.4e-03	-0.017350	102
C10	C13	4.312628	0.066750	0.068048	3.0e-03	-0.007350	103
C9	C12	4.312628	0.066750	0.068048	3.0e-03	-0.007350	103

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Table S10 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C13	H14	4.372455	0.123300	0.123754	5.6e-03	0.002700	102
C12	H15	4.372455	0.123300	0.123754	5.6e-03	0.002700	102
C2	H22	4.406496	0.189500	0.190197	8.5e-03	0.010800	102
C2	H23	4.406496	0.189500	0.190197	8.5e-03	0.010800	102
C2	H21	4.406495	0.189500	0.190197	8.5e-03	0.010800	102
C2	H20	4.406495	0.189500	0.190197	8.5e-03	0.010800	102
C4	H14	4.499615	0.103500	0.103881	4.7e-03	-0.014000	102
C3	H15	4.499615	0.103500	0.103881	4.7e-03	-0.014000	102
C5	H23	4.475973	0.219900	0.220709	9.9e-03	0.028000	102
C6	H22	4.475973	0.219900	0.220709	9.9e-03	0.028000	102
C6	H20	4.475973	0.219900	0.220709	9.9e-03	0.028000	102
C5	H21	4.475973	0.219900	0.220709	9.9e-03	0.028000	102
C4	H18	4.645705	0.102800	0.103178	4.6e-03	-0.015400	102
C3	H19	4.645705	0.102800	0.103178	4.6e-03	-0.015400	102
C10	H16	4.688561	0.105000	0.105386	4.7e-03	-0.018700	102
C9	H17	4.688561	0.105000	0.105386	4.7e-03	-0.018700	102
C9	C13	4.745571	0.065400	0.066671	2.9e-03	-0.000200	103
C10	C12	4.745571	0.065400	0.066671	2.9e-03	-0.000200	103
C8	C12	4.754566	0.067000	0.068302	3.0e-03	0.002600	103
C7	C13	4.754566	0.067000	0.068302	3.0e-03	0.002600	103
C5	C6	4.788722	0.061300	0.062492	2.8e-03	-0.012300	103
C13	H17	4.799354	0.106500	0.106892	4.8e-03	-0.018200	102
C12	H16	4.799354	0.106500	0.106892	4.8e-03	-0.018200	102
C7	C8	4.863587	0.063700	0.064938	2.9e-03	-0.014900	103
C9	H22	4.874297	0.167500	0.168116	7.5e-03	-0.003050	102
C10	H23	4.874297	0.167500	0.168116	7.5e-03	-0.003050	102
C9	H20	4.874297	0.167500	0.168116	7.5e-03	-0.003050	102
C10	H21	4.874297	0.167500	0.168116	7.5e-03	-0.003050	102
H16	H19	4.933930	0.163600	0.164202	7.4e-03	-0.019800	102
H18	H17	4.933930	0.163600	0.164202	7.4e-03	-0.019800	102
C6	H18	4.971611	0.118300	0.118735	5.3e-03	-0.017300	102
C5	H19	4.971611	0.118300	0.118735	5.3e-03	-0.017300	102
C5	C8	5.032471	0.065200	0.066467	2.9e-03	-0.014000	103
C6	C7	5.032471	0.065200	0.066467	2.9e-03	-0.014000	103
H15	H20	4.989739	0.245000	0.245901	1.1e-02	0.027200	102
H15	H22	4.989739	0.245000	0.245901	1.1e-02	0.027200	102
H14	H21	4.989739	0.245000	0.245901	1.1e-02	0.027200	102
H14	H23	4.989739	0.245000	0.245901	1.1e-02	0.027200	102
H17	H23	5.134083	0.171800	0.172432	7.7e-03	-0.025800	102
H17	H21	5.134083	0.171800	0.172432	7.7e-03	-0.025800	102
H16	H20	5.134083	0.171800	0.172432	7.7e-03	-0.025800	102
H16	H22	5.134083	0.171800	0.172432	7.7e-03	-0.025800	102
C4	H16	5.235353	0.094900	0.095249	4.3e-03	-0.016500	102
C3	H17	5.235353	0.094900	0.095249	4.3e-03	-0.016500	102
C9	H15	5.365623	0.096500	0.096855	4.3e-03	-0.018250	102
C10	H14	5.365623	0.096500	0.096855	4.3e-03	-0.018250	102
C12	H18	5.397838	0.097600	0.097959	4.4e-03	-0.011350	102
C13	H19	5.397838	0.097600	0.097959	4.4e-03	-0.011350	102
C10	H20	5.433506	0.222350	0.223168	1.0e-02	0.020000	102

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Table S10 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C9	H21	5.433506	0.222350	0.223168	1.0e-02	0.020000	102
C10	H22	5.433506	0.222350	0.223168	1.0e-02	0.020000	102
C9	H23	5.433506	0.222350	0.223168	1.0e-02	0.020000	102
C7	H21	5.448129	0.236050	0.236919	1.1e-02	0.027700	102
C8	H20	5.448129	0.236050	0.236919	1.1e-02	0.027700	102
C7	H23	5.448129	0.236050	0.236919	1.1e-02	0.027700	102
C8	H22	5.448129	0.236050	0.236919	1.1e-02	0.027700	102
C6	H14	5.745709	0.101800	0.102175	4.6e-03	-0.014300	102
C5	H15	5.745709	0.101800	0.102175	4.6e-03	-0.014300	102
C13	H18	5.765673	0.100500	0.100870	4.5e-03	-0.004200	102
C12	H19	5.765673	0.100500	0.100870	4.5e-03	-0.004200	102
C13	H16	5.783909	0.101400	0.101773	4.6e-03	-0.000400	102
C12	H17	5.783909	0.101400	0.101773	4.6e-03	-0.000400	102
C8	H16	5.852089	0.101700	0.102074	4.6e-03	-0.019000	102
C7	H17	5.852089	0.101700	0.102074	4.6e-03	-0.019000	102
H18	H20	5.943862	0.191450	0.192154	8.6e-03	-0.005125	102
H18	H22	5.943862	0.191450	0.192154	8.6e-03	-0.005125	102
H19	H21	5.943862	0.191450	0.192154	8.6e-03	-0.005125	102
H19	H23	5.943862	0.191450	0.192154	8.6e-03	-0.005125	102
H14	H19	6.043430	0.140400	0.140917	6.3e-03	-0.020600	102
H18	H15	6.043430	0.140400	0.140917	6.3e-03	-0.020600	102
C8	H14	6.089150	0.098650	0.099013	4.4e-03	-0.016700	102
C7	H15	6.089150	0.098650	0.099013	4.4e-03	-0.016700	102
C5	H17	6.103628	0.097900	0.098260	4.4e-03	-0.018000	102
C6	H16	6.103628	0.097900	0.098260	4.4e-03	-0.018000	102
H18	H21	6.431893	0.240750	0.241636	1.1e-02	0.016200	102
H19	H20	6.431893	0.240750	0.241636	1.1e-02	0.016200	102
H19	H22	6.431893	0.240750	0.241636	1.1e-02	0.016200	102
H18	H23	6.431893	0.240750	0.241636	1.1e-02	0.016200	102
H17	H20	6.459396	0.260375	0.261333	1.2e-02	0.027300	102
H17	H22	6.459396	0.260375	0.261333	1.2e-02	0.027300	102
H16	H21	6.459396	0.260375	0.261333	1.2e-02	0.027300	102
H16	H23	6.459396	0.260375	0.261333	1.2e-02	0.027300	102
H14	H15	6.646449	0.135600	0.136099	6.1e-03	-0.014500	102
H16	H17	6.797665	0.133000	0.133489	6.0e-03	-0.022000	102
H16	H15	7.165234	0.122350	0.122800	5.5e-03	-0.019400	102
H14	H17	7.165234	0.122350	0.122800	5.5e-03	-0.019400	102

Table S11: GED terms (in Å) for the GED(III) refinement.

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	H16	1.096141	0.075600	0.073055	2.2e-03	-0.015500	100
C8	H17	1.096141	0.075600	0.073055	2.2e-03	-0.015500	100
C5	H14	1.093768	0.075700	0.073152	2.2e-03	-0.015400	100
C6	H15	1.093768	0.075700	0.073152	2.2e-03	-0.015400	100
C9	H18	1.093820	0.075600	0.073055	2.2e-03	-0.015500	100

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Table S11 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C10	H19	1.093820	0.075600	0.073055	2.2e-03	-0.015500	100
C12	H20	1.103582	0.077100	0.074505	2.2e-03	-0.016800	100
C12	H22	1.103582	0.077100	0.074505	2.2e-03	-0.016800	100
C13	H21	1.103582	0.077100	0.074505	2.2e-03	-0.016800	100
C13	H23	1.103582	0.077100	0.074505	2.2e-03	-0.016800	100
C4	C6	1.367610	0.044100	0.048901	1.6e-03	-0.005600	101
C3	C5	1.367610	0.044100	0.048901	1.6e-03	-0.005600	101
C7	C9	1.385999	0.044600	0.049455	1.6e-03	-0.007700	101
C8	C10	1.385999	0.044600	0.049455	1.6e-03	-0.007700	101
C1	C3	1.412775	0.045700	0.050675	1.6e-03	-0.007150	101
C1	C4	1.412775	0.045700	0.050675	1.6e-03	-0.007150	101
C1	C2	1.402631	0.045500	0.050453	1.6e-03	-0.003700	101
C2	C10	1.428953	0.046600	0.051673	1.7e-03	-0.007500	101
C2	C9	1.428953	0.046600	0.051673	1.7e-03	-0.007500	101
C5	C7	1.437516	0.047100	0.052227	1.7e-03	-0.008200	101
C6	C8	1.437516	0.047100	0.052227	1.7e-03	-0.008200	101
C4	C13	1.519290	0.050900	0.056441	1.8e-03	-0.006500	101
C3	C12	1.519290	0.050900	0.056441	1.8e-03	-0.006500	101
C12	C13	1.564565	0.053700	0.059546	1.9e-03	-0.003400	101
H23	H21	1.749130	0.123600	0.124797	3.4e-03	-0.022300	102
H22	H20	1.749130	0.123600	0.124797	3.4e-03	-0.022300	102
C9	H16	2.146619	0.097600	0.098545	2.7e-03	-0.014000	102
C10	H17	2.146619	0.097600	0.098545	2.7e-03	-0.014000	102
C8	H19	2.151870	0.097600	0.098545	2.7e-03	-0.013600	102
C7	H18	2.151870	0.097600	0.098545	2.7e-03	-0.013600	102
C3	H14	2.148066	0.096700	0.097636	2.7e-03	-0.012300	102
C4	H15	2.148066	0.096700	0.097636	2.7e-03	-0.012300	102
C5	H16	2.179182	0.098900	0.099857	2.7e-03	-0.014200	102
C6	H17	2.179182	0.098900	0.099857	2.7e-03	-0.014200	102
C3	H20	2.179325	0.111000	0.112075	3.1e-03	-0.014500	102
C3	H22	2.179325	0.111000	0.112075	3.1e-03	-0.014500	102
C4	H23	2.179325	0.111000	0.112075	3.1e-03	-0.014500	102
C4	H21	2.179325	0.111000	0.112075	3.1e-03	-0.014500	102
C2	H19	2.171271	0.098500	0.099454	2.7e-03	-0.013800	102
C2	H18	2.171271	0.098500	0.099454	2.7e-03	-0.013800	102
C7	H14	2.190614	0.099000	0.099958	2.7e-03	-0.014600	102
C8	H15	2.190614	0.099000	0.099958	2.7e-03	-0.014600	102
C13	H22	2.219823	0.109700	0.110762	3.0e-03	-0.010700	102
C13	H20	2.219823	0.109700	0.110762	3.0e-03	-0.010700	102
C12	H23	2.219823	0.109700	0.110762	3.0e-03	-0.010700	102
C12	H21	2.219823	0.109700	0.110762	3.0e-03	-0.010700	102
C3	C4	2.337600	0.052900	0.058990	1.2e-03	-0.008800	103
H22	H21	2.406166	0.178500	0.180228	4.9e-03	-0.036700	102
H20	H23	2.406166	0.178500	0.180228	4.9e-03	-0.036700	102
C1	C12	2.383481	0.055300	0.061666	1.3e-03	-0.001300	103
C1	C13	2.383481	0.055300	0.061666	1.3e-03	-0.001300	103
C1	C6	2.398234	0.053600	0.059770	1.2e-03	-0.009800	103
C1	C5	2.398234	0.053600	0.059770	1.2e-03	-0.009800	103
C1	C9	2.394677	0.054900	0.061220	1.3e-03	-0.007600	103

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Table S11 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C1	C10	2.394677	0.054900	0.061220	1.3e-03	-0.007600	103
C3	C7	2.408130	0.054800	0.061108	1.3e-03	-0.008250	103
C4	C8	2.408130	0.054800	0.061108	1.3e-03	-0.008250	103
C2	C8	2.444875	0.054400	0.060662	1.3e-03	-0.010500	103
C2	C7	2.444875	0.054400	0.060662	1.3e-03	-0.010500	103
C3	C13	2.431513	0.058300	0.065011	1.3e-03	0.002450	103
C4	C12	2.431513	0.058300	0.065011	1.3e-03	0.002450	103
H16	H18	2.475640	0.158100	0.159631	4.4e-03	-0.012550	102
H19	H17	2.475640	0.158100	0.159631	4.4e-03	-0.012550	102
C6	C10	2.462909	0.054700	0.060997	1.3e-03	-0.011400	103
C5	C9	2.462909	0.054700	0.060997	1.3e-03	-0.011400	103
H14	H16	2.494972	0.159300	0.160842	4.4e-03	-0.014200	102
H17	H15	2.494972	0.159300	0.160842	4.4e-03	-0.014200	102
C2	C4	2.484944	0.055400	0.061777	1.3e-03	-0.007900	103
C2	C3	2.484944	0.055400	0.061777	1.3e-03	-0.007900	103
C9	C10	2.574375	0.059600	0.066461	1.4e-03	-0.011300	103
C5	C12	2.632333	0.062800	0.070029	1.4e-03	-0.012200	103
C6	C13	2.632333	0.062800	0.070029	1.4e-03	-0.012200	103
H18	H19	2.691670	0.185300	0.187094	5.1e-03	-0.013900	102
C1	C7	2.742669	0.059500	0.066349	1.4e-03	-0.009300	103
C1	C8	2.742669	0.059500	0.066349	1.4e-03	-0.009300	103
C3	C9	2.812771	0.060800	0.067799	1.4e-03	-0.009050	103
C4	C10	2.812771	0.060800	0.067799	1.4e-03	-0.009050	103
C10	H18	2.846537	0.128500	0.129744	3.6e-03	-0.013500	102
C9	H19	2.846537	0.128500	0.129744	3.6e-03	-0.013500	102
C2	C6	2.867118	0.060900	0.067911	1.4e-03	-0.011200	103
C2	C5	2.867118	0.060900	0.067911	1.4e-03	-0.011200	103
H20	H21	2.936747	0.167200	0.168819	4.6e-03	-0.004800	102
H22	H23	2.936747	0.167200	0.168819	4.6e-03	-0.004800	102
C13	H15	2.954064	0.129400	0.130653	3.6e-03	-0.018200	102
C12	H14	2.954064	0.129400	0.130653	3.6e-03	-0.018200	102
C5	H20	3.009289	0.137400	0.138730	3.8e-03	-0.023300	102
C5	H22	3.009290	0.137400	0.138730	3.8e-03	-0.023300	102
C6	H21	3.009289	0.137400	0.138730	3.8e-03	-0.023300	102
C6	H23	3.009290	0.137400	0.138730	3.8e-03	-0.023300	102
H14	H20	3.085360	0.219600	0.221726	6.1e-03	-0.029600	102
H15	H21	3.085360	0.219600	0.221726	6.1e-03	-0.029600	102
H15	H23	3.085360	0.219600	0.221726	6.1e-03	-0.029600	102
H14	H22	3.085360	0.219600	0.221726	6.1e-03	-0.029600	102
C1	H21	3.127826	0.169750	0.171393	4.7e-03	0.008350	102
C1	H22	3.127826	0.169750	0.171393	4.7e-03	0.008350	102
C1	H20	3.127826	0.169750	0.171393	4.7e-03	0.008350	102
C1	H23	3.127826	0.169750	0.171393	4.7e-03	0.008350	102
C4	H20	3.176445	0.184800	0.186589	5.1e-03	0.018000	102
C3	H21	3.176445	0.184800	0.186589	5.1e-03	0.018000	102
C4	H22	3.176445	0.184800	0.186589	5.1e-03	0.018000	102
C3	H23	3.176445	0.184800	0.186589	5.1e-03	0.018000	102
C4	H17	3.383177	0.094200	0.095112	2.6e-03	-0.014600	102
C3	H16	3.383177	0.094200	0.095112	2.6e-03	-0.014600	102

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Table S11 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C1	H14	3.398349	0.092900	0.093799	2.6e-03	-0.016050	102
C1	H15	3.398349	0.092900	0.093799	2.6e-03	-0.016050	102
C1	H18	3.381636	0.093700	0.094607	2.6e-03	-0.013400	102
C1	H19	3.381636	0.093700	0.094607	2.6e-03	-0.013400	102
C2	H17	3.429659	0.094100	0.095011	2.6e-03	-0.017000	102
C2	H16	3.429659	0.094100	0.095011	2.6e-03	-0.017000	102
C10	H15	3.434173	0.095000	0.095920	2.6e-03	-0.017600	102
C9	H14	3.434173	0.095000	0.095920	2.6e-03	-0.017600	102
C5	H18	3.447415	0.094600	0.095516	2.6e-03	-0.017500	102
C6	H19	3.447415	0.094600	0.095516	2.6e-03	-0.017500	102
C3	C6	3.609062	0.057900	0.064565	1.3e-03	-0.010600	103
C4	C5	3.609062	0.057900	0.064565	1.3e-03	-0.010600	103
C3	C10	3.730136	0.060000	0.066907	1.4e-03	-0.011300	103
C4	C9	3.730136	0.060000	0.066907	1.4e-03	-0.011300	103
C2	C13	3.733735	0.060900	0.067911	1.4e-03	-0.001600	103
C2	C12	3.733735	0.060900	0.067911	1.4e-03	-0.001600	103
C8	C9	3.802810	0.062700	0.069918	1.4e-03	-0.013900	103
C7	C10	3.802810	0.062700	0.069918	1.4e-03	-0.013900	103
C5	C13	3.777414	0.064600	0.072037	1.5e-03	0.004400	103
C6	C12	3.777414	0.064600	0.072037	1.5e-03	0.004400	103
C1	H17	3.829714	0.092400	0.093295	2.6e-03	-0.015750	102
C1	H16	3.829714	0.092400	0.093295	2.6e-03	-0.015750	102
C8	C13	3.883150	0.066000	0.073598	1.5e-03	-0.011850	103
C7	C12	3.883150	0.066000	0.073598	1.5e-03	-0.011850	103
C3	H18	3.897140	0.093300	0.094203	2.6e-03	-0.015150	102
C4	H19	3.897140	0.093300	0.094203	2.6e-03	-0.015150	102
C2	H14	3.951091	0.093400	0.094304	2.6e-03	-0.017200	102
C2	H15	3.951091	0.093400	0.094304	2.6e-03	-0.017200	102
C3	C8	4.144135	0.062900	0.070141	1.4e-03	-0.011700	103
C4	C7	4.144135	0.062900	0.070141	1.4e-03	-0.011700	103
C8	H18	4.209684	0.128000	0.129239	3.5e-03	-0.016150	102
C7	H19	4.209684	0.128000	0.129239	3.5e-03	-0.016150	102
C6	C9	4.282564	0.065100	0.072594	1.5e-03	-0.014100	103
C5	C10	4.282564	0.065100	0.072594	1.5e-03	-0.014100	103
H19	H15	4.327561	0.130600	0.131864	3.6e-03	-0.021600	102
H14	H18	4.327561	0.130600	0.131864	3.6e-03	-0.021600	102
C7	H22	4.317345	0.142100	0.143476	3.9e-03	-0.017350	102
C8	H23	4.317345	0.142100	0.143476	3.9e-03	-0.017350	102
C8	H21	4.317345	0.142100	0.143476	3.9e-03	-0.017350	102
C7	H20	4.317345	0.142100	0.143476	3.9e-03	-0.017350	102
C10	C13	4.301235	0.066750	0.074434	1.5e-03	-0.007350	103
C9	C12	4.301235	0.066750	0.074434	1.5e-03	-0.007350	103
C13	H14	4.347249	0.123300	0.124494	3.4e-03	0.002700	102
C12	H15	4.347249	0.123300	0.124494	3.4e-03	0.002700	102
C2	H22	4.410688	0.189500	0.191335	5.3e-03	0.010800	102
C2	H23	4.410688	0.189500	0.191335	5.3e-03	0.010800	102
C2	H21	4.410688	0.189500	0.191335	5.3e-03	0.010800	102
C2	H20	4.410688	0.189500	0.191335	5.3e-03	0.010800	102
C4	H14	4.478324	0.103500	0.104502	2.9e-03	-0.014000	102

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Table S11 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C3	H15	4.478324	0.103500	0.104502	2.9e-03	-0.014000	102
C5	H23	4.466854	0.219900	0.222029	6.1e-03	0.028000	102
C6	H22	4.466854	0.219900	0.222029	6.1e-03	0.028000	102
C6	H20	4.466854	0.219900	0.222029	6.1e-03	0.028000	102
C5	H21	4.466854	0.219900	0.222029	6.1e-03	0.028000	102
C4	H18	4.631224	0.102800	0.103795	2.8e-03	-0.015400	102
C3	H19	4.631224	0.102800	0.103795	2.8e-03	-0.015400	102
C10	H16	4.704458	0.105000	0.106017	2.9e-03	-0.018700	102
C9	H17	4.704458	0.105000	0.106017	2.9e-03	-0.018700	102
C9	C13	4.737165	0.065400	0.072929	1.5e-03	-0.000200	103
C10	C12	4.737165	0.065400	0.072929	1.5e-03	-0.000200	103
C8	C12	4.748608	0.067000	0.074713	1.5e-03	0.002600	103
C7	C13	4.748608	0.067000	0.074713	1.5e-03	0.002600	103
C5	C6	4.776065	0.061300	0.068357	1.4e-03	-0.012300	103
C13	H17	4.786189	0.106500	0.107531	3.0e-03	-0.018200	102
C12	H16	4.786189	0.106500	0.107531	3.0e-03	-0.018200	102
C7	C8	4.874740	0.063700	0.071033	1.5e-03	-0.014900	103
C9	H22	4.867625	0.167500	0.169122	4.6e-03	-0.003050	102
C10	H23	4.867625	0.167500	0.169122	4.6e-03	-0.003050	102
C9	H20	4.867625	0.167500	0.169122	4.6e-03	-0.003050	102
C10	H21	4.867625	0.167500	0.169122	4.6e-03	-0.003050	102
H16	H19	4.944642	0.163600	0.165184	4.5e-03	-0.019800	102
H18	H17	4.944642	0.163600	0.165184	4.5e-03	-0.019800	102
C6	H18	4.969126	0.118300	0.119445	3.3e-03	-0.017300	102
C5	H19	4.969126	0.118300	0.119445	3.3e-03	-0.017300	102
C5	C8	5.033371	0.065200	0.072706	1.5e-03	-0.014000	103
C6	C7	5.033371	0.065200	0.072706	1.5e-03	-0.014000	103
H15	H20	4.970273	0.245000	0.247372	6.8e-03	0.027200	102
H15	H22	4.970273	0.245000	0.247372	6.8e-03	0.027200	102
H14	H21	4.970273	0.245000	0.247372	6.8e-03	0.027200	102
H14	H23	4.970273	0.245000	0.247372	6.8e-03	0.027200	102
H17	H23	5.121018	0.171800	0.173463	4.8e-03	-0.025800	102
H17	H21	5.121018	0.171800	0.173463	4.8e-03	-0.025800	102
H16	H20	5.121018	0.171800	0.173463	4.8e-03	-0.025800	102
H16	H22	5.121018	0.171800	0.173463	4.8e-03	-0.025800	102
C4	H16	5.228447	0.094900	0.095819	2.6e-03	-0.016500	102
C3	H17	5.228447	0.094900	0.095819	2.6e-03	-0.016500	102
C9	H15	5.365001	0.096500	0.097434	2.7e-03	-0.018250	102
C10	H14	5.365001	0.096500	0.097434	2.7e-03	-0.018250	102
C12	H18	5.381805	0.097600	0.098545	2.7e-03	-0.011350	102
C13	H19	5.381805	0.097600	0.098545	2.7e-03	-0.011350	102
C10	H20	5.433183	0.222350	0.224503	6.2e-03	0.020000	102
C9	H21	5.433183	0.222350	0.224503	6.2e-03	0.020000	102
C10	H22	5.433183	0.222350	0.224503	6.2e-03	0.020000	102
C9	H23	5.433183	0.222350	0.224503	6.2e-03	0.020000	102
C7	H21	5.449999	0.236050	0.238335	6.5e-03	0.027700	102
C8	H20	5.449999	0.236050	0.238335	6.5e-03	0.027700	102
C7	H23	5.449999	0.236050	0.238335	6.5e-03	0.027700	102
C8	H22	5.449999	0.236050	0.238335	6.5e-03	0.027700	102

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Table S11 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C6	H14	5.724019	0.101800	0.102786	2.8e-03	-0.014300	102
C5	H15	5.724019	0.101800	0.102786	2.8e-03	-0.014300	102
C13	H18	5.750697	0.100500	0.101473	2.8e-03	-0.004200	102
C12	H19	5.750697	0.100500	0.101473	2.8e-03	-0.004200	102
C13	H16	5.774226	0.101400	0.102382	2.8e-03	-0.000400	102
C12	H17	5.774226	0.101400	0.102382	2.8e-03	-0.000400	102
C8	H16	5.864986	0.101700	0.102685	2.8e-03	-0.019000	102
C7	H17	5.864986	0.101700	0.102685	2.8e-03	-0.019000	102
H18	H20	5.933515	0.191450	0.193303	5.3e-03	-0.005125	102
H18	H22	5.933515	0.191450	0.193303	5.3e-03	-0.005125	102
H19	H21	5.933515	0.191450	0.193303	5.3e-03	-0.005125	102
H19	H23	5.933515	0.191450	0.193303	5.3e-03	-0.005125	102
H14	H19	6.038322	0.140400	0.141759	3.9e-03	-0.020600	102
H18	H15	6.038322	0.140400	0.141759	3.9e-03	-0.020600	102
C8	H14	6.083585	0.098650	0.099605	2.7e-03	-0.016700	102
C7	H15	6.083585	0.098650	0.099605	2.7e-03	-0.016700	102
C5	H17	6.104244	0.097900	0.098848	2.7e-03	-0.018000	102
C6	H16	6.104244	0.097900	0.098848	2.7e-03	-0.018000	102
H18	H21	6.425127	0.240750	0.243081	6.7e-03	0.016200	102
H19	H20	6.425127	0.240750	0.243081	6.7e-03	0.016200	102
H19	H22	6.425127	0.240750	0.243081	6.7e-03	0.016200	102
H18	H23	6.425127	0.240750	0.243081	6.7e-03	0.016200	102
H17	H20	6.457646	0.260375	0.262896	7.2e-03	0.027300	102
H17	H22	6.457646	0.260375	0.262896	7.2e-03	0.027300	102
H16	H21	6.457646	0.260375	0.262896	7.2e-03	0.027300	102
H16	H23	6.457646	0.260375	0.262896	7.2e-03	0.027300	102
H14	H15	6.613906	0.135600	0.136913	3.8e-03	-0.014500	102
H16	H17	6.813944	0.133000	0.134288	3.7e-03	-0.022000	102
H16	H15	7.159220	0.122350	0.123535	3.4e-03	-0.019400	102
H14	H17	7.159220	0.122350	0.123535	3.4e-03	-0.019400	102

Table S12: GED terms (in Å) for the GED+MW(IV) refinement.

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	H16	1.097606	0.075600	0.075813	3.6e-03	-0.015500	100
C8	H17	1.097606	0.075600	0.075813	3.6e-03	-0.015500	100
C5	H14	1.097487	0.075700	0.075913	3.6e-03	-0.015400	100
C6	H15	1.097487	0.075700	0.075913	3.6e-03	-0.015400	100
C9	H18	1.097653	0.075600	0.075813	3.6e-03	-0.015500	100
C10	H19	1.097653	0.075600	0.075813	3.6e-03	-0.015500	100
C12	H20	1.107936	0.077100	0.077317	3.7e-03	-0.016800	100
C12	H22	1.107936	0.077100	0.077317	3.7e-03	-0.016800	100
C13	H21	1.107936	0.077100	0.077317	3.7e-03	-0.016800	100
C13	H23	1.107936	0.077100	0.077317	3.7e-03	-0.016800	100
C4	C6	1.375277	0.044100	0.044771	2.0e-03	-0.005600	101
C3	C5	1.375277	0.044100	0.044771	2.0e-03	-0.005600	101

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Table S12 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	C9	1.386957	0.044600	0.045279	2.0e-03	-0.007700	101
C8	C10	1.386957	0.044600	0.045279	2.0e-03	-0.007700	101
C1	C3	1.414134	0.045700	0.046396	2.0e-03	-0.007150	101
C1	C4	1.414134	0.045700	0.046396	2.0e-03	-0.007150	101
C1	C2	1.405840	0.045500	0.046193	2.0e-03	-0.003700	101
C2	C10	1.425450	0.046600	0.047309	2.1e-03	-0.007500	101
C2	C9	1.425450	0.046600	0.047309	2.1e-03	-0.007500	101
C5	C7	1.431005	0.047100	0.047817	2.1e-03	-0.008200	101
C6	C8	1.431005	0.047100	0.047817	2.1e-03	-0.008200	101
C4	C13	1.518251	0.050900	0.051675	2.3e-03	-0.006500	101
C3	C12	1.518251	0.050900	0.051675	2.3e-03	-0.006500	101
C12	C13	1.566615	0.053700	0.054517	2.4e-03	-0.003400	101
H23	H21	1.778698	0.123600	0.125127	5.6e-03	-0.022300	102
H22	H20	1.778698	0.123600	0.125127	5.6e-03	-0.022300	102
C9	H16	2.140333	0.097600	0.098806	4.4e-03	-0.014000	102
C10	H17	2.140333	0.097600	0.098806	4.4e-03	-0.014000	102
C8	H19	2.152743	0.097600	0.098806	4.4e-03	-0.013600	102
C7	H18	2.152743	0.097600	0.098806	4.4e-03	-0.013600	102
C3	H14	2.158291	0.096700	0.097895	4.4e-03	-0.012300	102
C4	H15	2.158291	0.096700	0.097895	4.4e-03	-0.012300	102
C5	H16	2.174907	0.098900	0.100122	4.5e-03	-0.014200	102
C6	H17	2.174907	0.098900	0.100122	4.5e-03	-0.014200	102
C3	H20	2.174512	0.111000	0.112372	5.0e-03	-0.014500	102
C3	H22	2.174512	0.111000	0.112372	5.0e-03	-0.014500	102
C4	H23	2.174512	0.111000	0.112372	5.0e-03	-0.014500	102
C4	H21	2.174512	0.111000	0.112372	5.0e-03	-0.014500	102
C2	H19	2.183003	0.098500	0.099717	4.5e-03	-0.013800	102
C2	H18	2.183003	0.098500	0.099717	4.5e-03	-0.013800	102
C7	H14	2.187502	0.099000	0.100223	4.5e-03	-0.014600	102
C8	H15	2.187502	0.099000	0.100223	4.5e-03	-0.014600	102
C13	H22	2.218752	0.109700	0.111056	5.0e-03	-0.010700	102
C13	H20	2.218752	0.109700	0.111056	5.0e-03	-0.010700	102
C12	H23	2.218752	0.109700	0.111056	5.0e-03	-0.010700	102
C12	H21	2.218752	0.109700	0.111056	5.0e-03	-0.010700	102
C3	C4	2.342701	0.052900	0.053712	2.2e-03	-0.008800	103
H22	H21	2.393968	0.178500	0.180706	8.1e-03	-0.036700	102
H20	H23	2.393968	0.178500	0.180706	8.1e-03	-0.036700	102
C1	C12	2.381148	0.055300	0.056149	2.3e-03	-0.001300	103
C1	C13	2.381148	0.055300	0.056149	2.3e-03	-0.001300	103
C1	C6	2.400122	0.053600	0.054423	2.3e-03	-0.009800	103
C1	C5	2.400122	0.053600	0.054423	2.3e-03	-0.009800	103
C1	C9	2.402329	0.054900	0.055743	2.3e-03	-0.007600	103
C1	C10	2.402329	0.054900	0.055743	2.3e-03	-0.007600	103
C3	C7	2.409157	0.054800	0.055641	2.3e-03	-0.008250	103
C4	C8	2.409157	0.054800	0.055641	2.3e-03	-0.008250	103
C2	C8	2.433128	0.054400	0.055235	2.3e-03	-0.010500	103
C2	C7	2.433128	0.054400	0.055235	2.3e-03	-0.010500	103
C3	C13	2.433485	0.058300	0.059195	2.5e-03	0.002450	103
C4	C12	2.433485	0.058300	0.059195	2.5e-03	0.002450	103

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Table S12 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
H16	H18	2.461436	0.158100	0.160054	7.2e-03	-0.012550	102
H19	H17	2.461436	0.158100	0.160054	7.2e-03	-0.012550	102
C6	C10	2.466912	0.054700	0.055540	2.3e-03	-0.011400	103
C5	C9	2.466912	0.054700	0.055540	2.3e-03	-0.011400	103
H14	H16	2.491122	0.159300	0.161269	7.2e-03	-0.014200	102
H17	H15	2.491122	0.159300	0.161269	7.2e-03	-0.014200	102
C2	C4	2.487785	0.055400	0.056251	2.4e-03	-0.007900	103
C2	C3	2.487785	0.055400	0.056251	2.4e-03	-0.007900	103
C9	C10	2.554931	0.059600	0.060515	2.5e-03	-0.011300	103
C5	C12	2.644982	0.062800	0.063764	2.7e-03	-0.012200	103
C6	C13	2.644982	0.062800	0.063764	2.7e-03	-0.012200	103
H18	H19	2.690778	0.185300	0.187590	8.4e-03	-0.013900	102
C1	C7	2.737739	0.059500	0.060413	2.5e-03	-0.009300	103
C1	C8	2.737739	0.059500	0.060413	2.5e-03	-0.009300	103
C3	C9	2.826116	0.060800	0.061733	2.6e-03	-0.009050	103
C4	C10	2.826116	0.060800	0.061733	2.6e-03	-0.009050	103
C10	H18	2.838397	0.128500	0.130088	5.8e-03	-0.013500	102
C9	H19	2.838397	0.128500	0.130088	5.8e-03	-0.013500	102
C2	C6	2.862027	0.060900	0.061835	2.6e-03	-0.011200	103
C2	C5	2.862027	0.060900	0.061835	2.6e-03	-0.011200	103
H20	H21	2.944468	0.167200	0.169266	7.6e-03	-0.004800	102
H22	H23	2.944468	0.167200	0.169266	7.6e-03	-0.004800	102
C13	H15	2.974983	0.129400	0.130999	5.9e-03	-0.018200	102
C12	H14	2.974983	0.129400	0.130999	5.9e-03	-0.018200	102
C5	H20	3.020889	0.137400	0.139098	6.2e-03	-0.023300	102
C5	H22	3.020889	0.137400	0.139098	6.2e-03	-0.023300	102
C6	H21	3.020889	0.137400	0.139098	6.2e-03	-0.023300	102
C6	H23	3.020889	0.137400	0.139098	6.2e-03	-0.023300	102
H14	H20	3.110062	0.219600	0.222314	1.0e-02	-0.029600	102
H15	H21	3.110062	0.219600	0.222314	1.0e-02	-0.029600	102
H15	H23	3.110062	0.219600	0.222314	1.0e-02	-0.029600	102
H14	H22	3.110062	0.219600	0.222314	1.0e-02	-0.029600	102
C1	H21	3.118115	0.169750	0.171848	7.7e-03	0.008350	102
C1	H22	3.118115	0.169750	0.171848	7.7e-03	0.008350	102
C1	H20	3.118115	0.169750	0.171848	7.7e-03	0.008350	102
C1	H23	3.118115	0.169750	0.171848	7.7e-03	0.008350	102
C4	H20	3.170618	0.184800	0.187084	8.4e-03	0.018000	102
C3	H21	3.170618	0.184800	0.187084	8.4e-03	0.018000	102
C4	H22	3.170618	0.184800	0.187084	8.4e-03	0.018000	102
C3	H23	3.170618	0.184800	0.187084	8.4e-03	0.018000	102
C4	H17	3.386974	0.094200	0.095364	4.3e-03	-0.014600	102
C3	H16	3.386974	0.094200	0.095364	4.3e-03	-0.014600	102
C1	H14	3.404851	0.092900	0.094048	4.2e-03	-0.016050	102
C1	H15	3.404851	0.092900	0.094048	4.2e-03	-0.016050	102
C1	H18	3.398439	0.093700	0.094858	4.3e-03	-0.013400	102
C1	H19	3.398439	0.093700	0.094858	4.3e-03	-0.013400	102
C2	H17	3.416464	0.094100	0.095263	4.3e-03	-0.017000	102
C2	H16	3.416464	0.094100	0.095263	4.3e-03	-0.017000	102
C10	H15	3.439346	0.095000	0.096174	4.3e-03	-0.017600	102

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Table S12 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C9	H14	3.439346	0.095000	0.096174	4.3e-03	-0.017600	102
C5	H18	3.449742	0.094600	0.095769	4.3e-03	-0.017500	102
C6	H19	3.449742	0.094600	0.095769	4.3e-03	-0.017500	102
C3	C6	3.617353	0.057900	0.058789	2.5e-03	-0.010600	103
C4	C5	3.617353	0.057900	0.058789	2.5e-03	-0.010600	103
C3	C10	3.735873	0.060000	0.060921	2.5e-03	-0.011300	103
C4	C9	3.735873	0.060000	0.060921	2.5e-03	-0.011300	103
C2	C13	3.734325	0.060900	0.061835	2.6e-03	-0.001600	103
C2	C12	3.734325	0.060900	0.061835	2.6e-03	-0.001600	103
C8	C9	3.783050	0.062700	0.063663	2.7e-03	-0.013900	103
C7	C10	3.783050	0.062700	0.063663	2.7e-03	-0.013900	103
C5	C13	3.788757	0.064600	0.065592	2.7e-03	0.004400	103
C6	C12	3.788757	0.064600	0.065592	2.7e-03	0.004400	103
C1	H17	3.826282	0.092400	0.093542	4.2e-03	-0.015750	102
C1	H16	3.826282	0.092400	0.093542	4.2e-03	-0.015750	102
C8	C13	3.885400	0.066000	0.067013	2.8e-03	-0.011850	103
C7	C12	3.885400	0.066000	0.067013	2.8e-03	-0.011850	103
C3	H18	3.914136	0.093300	0.094453	4.2e-03	-0.015150	102
C4	H19	3.914136	0.093300	0.094453	4.2e-03	-0.015150	102
C2	H14	3.949562	0.093400	0.094554	4.2e-03	-0.017200	102
C2	H15	3.949562	0.093400	0.094554	4.2e-03	-0.017200	102
C3	C8	4.141347	0.062900	0.063866	2.7e-03	-0.011700	103
C4	C7	4.141347	0.062900	0.063866	2.7e-03	-0.011700	103
C8	H18	4.202392	0.128000	0.129582	5.8e-03	-0.016150	102
C7	H19	4.202392	0.128000	0.129582	5.8e-03	-0.016150	102
C6	C9	4.275860	0.065100	0.066099	2.8e-03	-0.014100	103
C5	C10	4.275860	0.065100	0.066099	2.8e-03	-0.014100	103
H19	H15	4.327626	0.130600	0.132214	5.9e-03	-0.021600	102
H14	H18	4.327626	0.130600	0.132214	5.9e-03	-0.021600	102
C7	H22	4.317005	0.142100	0.143856	6.5e-03	-0.017350	102
C8	H23	4.317005	0.142100	0.143856	6.5e-03	-0.017350	102
C8	H21	4.317005	0.142100	0.143856	6.5e-03	-0.017350	102
C7	H20	4.317005	0.142100	0.143856	6.5e-03	-0.017350	102
C10	C13	4.312279	0.066750	0.067775	2.8e-03	-0.007350	103
C9	C12	4.312279	0.066750	0.067775	2.8e-03	-0.007350	103
C13	H14	4.367298	0.123300	0.124824	5.6e-03	0.002700	102
C12	H15	4.367298	0.123300	0.124824	5.6e-03	0.002700	102
C2	H22	4.402697	0.189500	0.191842	8.6e-03	0.010800	102
C2	H23	4.402697	0.189500	0.191842	8.6e-03	0.010800	102
C2	H21	4.402697	0.189500	0.191842	8.6e-03	0.010800	102
C2	H20	4.402697	0.189500	0.191842	8.6e-03	0.010800	102
C4	H14	4.493330	0.103500	0.104779	4.7e-03	-0.014000	102
C3	H15	4.493330	0.103500	0.104779	4.7e-03	-0.014000	102
C5	H23	4.469739	0.219900	0.222618	1.0e-02	0.028000	102
C6	H22	4.469739	0.219900	0.222618	1.0e-02	0.028000	102
C6	H20	4.469739	0.219900	0.222618	1.0e-02	0.028000	102
C5	H21	4.469739	0.219900	0.222618	1.0e-02	0.028000	102
C4	H18	4.646778	0.102800	0.104070	4.7e-03	-0.015400	102
C3	H19	4.646778	0.102800	0.104070	4.7e-03	-0.015400	102

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Table S12 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C10	H16	4.679201	0.105000	0.106298	4.8e-03	-0.018700	102
C9	H17	4.679201	0.105000	0.106298	4.8e-03	-0.018700	102
C9	C13	4.744529	0.065400	0.066404	2.8e-03	-0.000200	103
C10	C12	4.744529	0.065400	0.066404	2.8e-03	-0.000200	103
C8	C12	4.747772	0.067000	0.068029	2.8e-03	0.002600	103
C7	C13	4.747772	0.067000	0.068029	2.8e-03	0.002600	103
C5	C6	4.782276	0.061300	0.062241	2.6e-03	-0.012300	103
C13	H17	4.793356	0.106500	0.107816	4.8e-03	-0.018200	102
C12	H16	4.793356	0.106500	0.107816	4.8e-03	-0.018200	102
C7	C8	4.852134	0.063700	0.064678	2.7e-03	-0.014900	103
C9	H22	4.872312	0.167500	0.169570	7.6e-03	-0.003050	102
C10	H23	4.872312	0.167500	0.169570	7.6e-03	-0.003050	102
C9	H20	4.872312	0.167500	0.169570	7.6e-03	-0.003050	102
C10	H21	4.872312	0.167500	0.169570	7.6e-03	-0.003050	102
H16	H19	4.928667	0.163600	0.165622	7.4e-03	-0.019800	102
H18	H17	4.928667	0.163600	0.165622	7.4e-03	-0.019800	102
C6	H18	4.971988	0.118300	0.119762	5.4e-03	-0.017300	102
C5	H19	4.971988	0.118300	0.119762	5.4e-03	-0.017300	102
C5	C8	5.023777	0.065200	0.066201	2.8e-03	-0.014000	103
C6	C7	5.023777	0.065200	0.066201	2.8e-03	-0.014000	103
H15	H20	4.983104	0.245000	0.248028	1.1e-02	0.027200	102
H15	H22	4.983104	0.245000	0.248028	1.1e-02	0.027200	102
H14	H21	4.983104	0.245000	0.248028	1.1e-02	0.027200	102
H14	H23	4.983104	0.245000	0.248028	1.1e-02	0.027200	102
H17	H23	5.127502	0.171800	0.173923	7.8e-03	-0.025800	102
H17	H21	5.127502	0.171800	0.173923	7.8e-03	-0.025800	102
H16	H20	5.127502	0.171800	0.173923	7.8e-03	-0.025800	102
H16	H22	5.127502	0.171800	0.173923	7.8e-03	-0.025800	102
C4	H16	5.227428	0.094900	0.096073	4.3e-03	-0.016500	102
C3	H17	5.227428	0.094900	0.096073	4.3e-03	-0.016500	102
C9	H15	5.362094	0.096500	0.097693	4.4e-03	-0.018250	102
C10	H14	5.362094	0.096500	0.097693	4.4e-03	-0.018250	102
C12	H18	5.397239	0.097600	0.098806	4.4e-03	-0.011350	102
C13	H19	5.397239	0.097600	0.098806	4.4e-03	-0.011350	102
C10	H20	5.430296	0.222350	0.225098	1.0e-02	0.020000	102
C9	H21	5.430296	0.222350	0.225098	1.0e-02	0.020000	102
C10	H22	5.430297	0.222350	0.225098	1.0e-02	0.020000	102
C9	H23	5.430297	0.222350	0.225098	1.0e-02	0.020000	102
C7	H21	5.439447	0.236050	0.238967	1.1e-02	0.027700	102
C8	H20	5.439447	0.236050	0.238967	1.1e-02	0.027700	102
C7	H23	5.439447	0.236050	0.238967	1.1e-02	0.027700	102
C8	H22	5.439447	0.236050	0.238967	1.1e-02	0.027700	102
C6	H14	5.738453	0.101800	0.103058	4.6e-03	-0.014300	102
C5	H15	5.738453	0.101800	0.103058	4.6e-03	-0.014300	102
C13	H18	5.765479	0.100500	0.101742	4.6e-03	-0.004200	102
C12	H19	5.765479	0.100500	0.101742	4.6e-03	-0.004200	102
C13	H16	5.777244	0.101400	0.102653	4.6e-03	-0.000400	102
C12	H17	5.777244	0.101400	0.102653	4.6e-03	-0.000400	102
C8	H16	5.839508	0.101700	0.102957	4.6e-03	-0.019000	102

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Table S12 – continued from the previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	H17	5.839508	0.101700	0.102957	4.6e-03	-0.019000	102
H18	H20	5.941227	0.191450	0.193816	8.7e-03	-0.005125	102
H18	H22	5.941227	0.191450	0.193816	8.7e-03	-0.005125	102
H19	H21	5.941227	0.191450	0.193816	8.7e-03	-0.005125	102
H19	H23	5.941227	0.191450	0.193816	8.7e-03	-0.005125	102
H14	H19	6.043288	0.140400	0.142135	6.4e-03	-0.020600	102
H18	H15	6.043288	0.140400	0.142135	6.4e-03	-0.020600	102
C8	H14	6.079869	0.098650	0.099869	4.5e-03	-0.016700	102
C7	H15	6.079869	0.098650	0.099869	4.5e-03	-0.016700	102
C5	H17	6.094285	0.097900	0.099110	4.5e-03	-0.018000	102
C6	H16	6.094285	0.097900	0.099110	4.5e-03	-0.018000	102
H18	H21	6.429530	0.240750	0.243725	1.1e-02	0.016200	102
H19	H20	6.429530	0.240750	0.243725	1.1e-02	0.016200	102
H19	H22	6.429530	0.240750	0.243725	1.1e-02	0.016200	102
H18	H23	6.429530	0.240750	0.243725	1.1e-02	0.016200	102
H17	H20	6.450835	0.260375	0.263593	1.2e-02	0.027300	102
H17	H22	6.450835	0.260375	0.263593	1.2e-02	0.027300	102
H16	H21	6.450835	0.260375	0.263593	1.2e-02	0.027300	102
H16	H23	6.450835	0.260375	0.263593	1.2e-02	0.027300	102
H14	H15	6.638227	0.135600	0.137276	6.2e-03	-0.014500	102
H16	H17	6.783583	0.133000	0.134644	6.0e-03	-0.022000	102
H16	H15	7.155367	0.122350	0.123862	5.6e-03	-0.019400	102
H14	H17	7.155367	0.122350	0.123862	5.6e-03	-0.019400	102

Table S13: GED terms (in Å) for the GED+MW(V) refinement.

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C7	H16	1.096383	0.075600	0.072630	2.2e-03	-0.015500	100
C8	H17	1.096383	0.075600	0.072630	2.2e-03	-0.015500	100
C5	H14	1.093786	0.075700	0.072726	2.2e-03	-0.015400	100
C6	H15	1.093786	0.075700	0.072726	2.2e-03	-0.015400	100
C9	H18	1.094246	0.075600	0.072630	2.2e-03	-0.015500	100
C10	H19	1.094246	0.075600	0.072630	2.2e-03	-0.015500	100
C12	H20	1.109213	0.077100	0.074071	2.2e-03	-0.016800	100
C12	H22	1.109213	0.077100	0.074071	2.2e-03	-0.016800	100
C13	H21	1.109213	0.077100	0.074071	2.2e-03	-0.016800	100
C13	H23	1.109213	0.077100	0.074071	2.2e-03	-0.016800	100
C4	C6	1.367667	0.044100	0.048563	1.5e-03	-0.005600	101
C3	C5	1.367667	0.044100	0.048563	1.5e-03	-0.005600	101
C7	C9	1.385297	0.044600	0.049113	1.6e-03	-0.007700	101
C8	C10	1.385297	0.044600	0.049113	1.6e-03	-0.007700	101
C1	C3	1.413104	0.045700	0.050324	1.6e-03	-0.007150	101
C1	C4	1.413104	0.045700	0.050324	1.6e-03	-0.007150	101
C1	C2	1.403724	0.045500	0.050104	1.6e-03	-0.003700	101
C2	C10	1.428408	0.046600	0.051316	1.6e-03	-0.007500	101
C2	C9	1.428408	0.046600	0.051316	1.6e-03	-0.007500	101

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Table S13 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C5	C7	1.438164	0.047100	0.051866	1.7e-03	-0.008200	101
C6	C8	1.438164	0.047100	0.051866	1.7e-03	-0.008200	101
C4	C13	1.521833	0.050900	0.056051	1.8e-03	-0.006500	101
C3	C12	1.521833	0.050900	0.056051	1.8e-03	-0.006500	101
C12	C13	1.563411	0.053700	0.059134	1.9e-03	-0.003400	101
H23	H21	1.773003	0.123600	0.124504	3.6e-03	-0.022300	102
H22	H20	1.773003	0.123600	0.124504	3.6e-03	-0.022300	102
C9	H16	2.142570	0.097600	0.098314	2.8e-03	-0.014000	102
C10	H17	2.142570	0.097600	0.098314	2.8e-03	-0.014000	102
C8	H19	2.151594	0.097600	0.098314	2.8e-03	-0.013600	102
C7	H18	2.151594	0.097600	0.098314	2.8e-03	-0.013600	102
C3	H14	2.147831	0.096700	0.097407	2.8e-03	-0.012300	102
C4	H15	2.147831	0.096700	0.097407	2.8e-03	-0.012300	102
C5	H16	2.180587	0.098900	0.099623	2.9e-03	-0.014200	102
C6	H17	2.180587	0.098900	0.099623	2.9e-03	-0.014200	102
C3	H20	2.183243	0.111000	0.111812	3.2e-03	-0.014500	102
C3	H22	2.183243	0.111000	0.111812	3.2e-03	-0.014500	102
C4	H23	2.183243	0.111000	0.111812	3.2e-03	-0.014500	102
C4	H21	2.183243	0.111000	0.111812	3.2e-03	-0.014500	102
C2	H19	2.176748	0.098500	0.099220	2.8e-03	-0.013800	102
C2	H18	2.176748	0.098500	0.099220	2.8e-03	-0.013800	102
C7	H14	2.190241	0.099000	0.099724	2.9e-03	-0.014600	102
C8	H15	2.190241	0.099000	0.099724	2.9e-03	-0.014600	102
C13	H22	2.216806	0.109700	0.110502	3.2e-03	-0.010700	102
C13	H20	2.216806	0.109700	0.110502	3.2e-03	-0.010700	102
C12	H23	2.216806	0.109700	0.110502	3.2e-03	-0.010700	102
C12	H21	2.216806	0.109700	0.110502	3.2e-03	-0.010700	102
C3	C4	2.340664	0.052900	0.059867	1.2e-03	-0.008800	103
H22	H21	2.391516	0.178500	0.179805	5.2e-03	-0.036700	102
H20	H23	2.391516	0.178500	0.179805	5.2e-03	-0.036700	102
C1	C12	2.383664	0.055300	0.062583	1.3e-03	-0.001300	103
C1	C13	2.383664	0.055300	0.062583	1.3e-03	-0.001300	103
C1	C6	2.395752	0.053600	0.060659	1.2e-03	-0.009800	103
C1	C5	2.395752	0.053600	0.060659	1.2e-03	-0.009800	103
C1	C9	2.400846	0.054900	0.062130	1.2e-03	-0.007600	103
C1	C10	2.400846	0.054900	0.062130	1.2e-03	-0.007600	103
C3	C7	2.410232	0.054800	0.062017	1.2e-03	-0.008250	103
C4	C8	2.410232	0.054800	0.062017	1.2e-03	-0.008250	103
C2	C8	2.437512	0.054400	0.061565	1.2e-03	-0.010500	103
C2	C7	2.437512	0.054400	0.061565	1.2e-03	-0.010500	103
C3	C13	2.433523	0.058300	0.065978	1.3e-03	0.002450	103
C4	C12	2.433523	0.058300	0.065978	1.3e-03	0.002450	103
H16	H18	2.469694	0.158100	0.159256	4.6e-03	-0.012550	102
H19	H17	2.469694	0.158100	0.159256	4.6e-03	-0.012550	102
C6	C10	2.466253	0.054700	0.061904	1.2e-03	-0.011400	103
C5	C9	2.466253	0.054700	0.061904	1.2e-03	-0.011400	103
H14	H16	2.495206	0.159300	0.160465	4.6e-03	-0.014200	102
H17	H15	2.495206	0.159300	0.160465	4.6e-03	-0.014200	102
C2	C4	2.485145	0.055400	0.062696	1.3e-03	-0.007900	103

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Table S13 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C2	C3	2.485145	0.055400	0.062696	1.3e-03	-0.007900	103
C9	C10	2.563948	0.059600	0.067450	1.4e-03	-0.011300	103
C5	C12	2.638624	0.062800	0.071071	1.4e-03	-0.012200	103
C6	C13	2.638624	0.062800	0.071071	1.4e-03	-0.012200	103
H18	H19	2.684363	0.185300	0.186655	5.4e-03	-0.013900	102
C1	C7	2.740851	0.059500	0.067336	1.3e-03	-0.009300	103
C1	C8	2.740851	0.059500	0.067336	1.3e-03	-0.009300	103
C3	C9	2.821414	0.060800	0.068808	1.4e-03	-0.009050	103
C4	C10	2.821414	0.060800	0.068808	1.4e-03	-0.009050	103
C10	H18	2.838468	0.128500	0.129439	3.7e-03	-0.013500	102
C9	H19	2.838468	0.128500	0.129439	3.7e-03	-0.013500	102
C2	C6	2.861452	0.060900	0.068921	1.4e-03	-0.011200	103
C2	C5	2.861452	0.060900	0.068921	1.4e-03	-0.011200	103
H20	H21	2.939101	0.167200	0.168422	4.8e-03	-0.004800	102
H22	H23	2.939101	0.167200	0.168422	4.8e-03	-0.004800	102
C13	H15	2.962456	0.129400	0.130346	3.7e-03	-0.018200	102
C12	H14	2.962456	0.129400	0.130346	3.7e-03	-0.018200	102
C5	H20	3.020143	0.137400	0.138405	4.0e-03	-0.023300	102
C5	H22	3.020143	0.137400	0.138405	4.0e-03	-0.023300	102
C6	H21	3.020143	0.137400	0.138405	4.0e-03	-0.023300	102
C6	H23	3.020143	0.137400	0.138405	4.0e-03	-0.023300	102
H14	H20	3.101608	0.219600	0.221205	6.3e-03	-0.029600	102
H15	H21	3.101608	0.219600	0.221205	6.3e-03	-0.029600	102
H15	H23	3.101608	0.219600	0.221205	6.3e-03	-0.029600	102
H14	H22	3.101608	0.219600	0.221205	6.3e-03	-0.029600	102
C1	H21	3.126113	0.169750	0.170991	4.9e-03	0.008350	102
C1	H22	3.126113	0.169750	0.170991	4.9e-03	0.008350	102
C1	H20	3.126113	0.169750	0.170991	4.9e-03	0.008350	102
C1	H23	3.126113	0.169750	0.170991	4.9e-03	0.008350	102
C4	H20	3.174892	0.184800	0.186151	5.3e-03	0.018000	102
C3	H21	3.174892	0.184800	0.186151	5.3e-03	0.018000	102
C4	H22	3.174892	0.184800	0.186151	5.3e-03	0.018000	102
C3	H23	3.174892	0.184800	0.186151	5.3e-03	0.018000	102
C4	H17	3.385419	0.094200	0.094889	2.7e-03	-0.014600	102
C3	H16	3.385419	0.094200	0.094889	2.7e-03	-0.014600	102
C1	H14	3.396469	0.092900	0.093579	2.7e-03	-0.016050	102
C1	H15	3.396469	0.092900	0.093579	2.7e-03	-0.016050	102
C1	H18	3.390236	0.093700	0.094385	2.7e-03	-0.013400	102
C1	H19	3.390236	0.093700	0.094385	2.7e-03	-0.013400	102
C2	H17	3.422112	0.094100	0.094788	2.7e-03	-0.017000	102
C2	H16	3.422112	0.094100	0.094788	2.7e-03	-0.017000	102
C10	H15	3.435746	0.095000	0.095695	2.7e-03	-0.017600	102
C9	H14	3.435746	0.095000	0.095695	2.7e-03	-0.017600	102
C5	H18	3.450247	0.094600	0.095292	2.7e-03	-0.017500	102
C6	H19	3.450247	0.094600	0.095292	2.7e-03	-0.017500	102
C3	C6	3.609899	0.057900	0.065526	1.3e-03	-0.010600	103
C4	C5	3.609899	0.057900	0.065526	1.3e-03	-0.010600	103
C3	C10	3.734446	0.060000	0.067902	1.4e-03	-0.011300	103
C4	C9	3.734446	0.060000	0.067902	1.4e-03	-0.011300	103

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Table S13 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C2	C13	3.735069	0.060900	0.068921	1.4e-03	-0.001600	103
C2	C12	3.735069	0.060900	0.068921	1.4e-03	-0.001600	103
C8	C9	3.791209	0.062700	0.070958	1.4e-03	-0.013900	103
C7	C10	3.791209	0.062700	0.070958	1.4e-03	-0.013900	103
C5	C13	3.780279	0.064600	0.073108	1.5e-03	0.004400	103
C6	C12	3.780279	0.064600	0.073108	1.5e-03	0.004400	103
C1	H17	3.828140	0.092400	0.093076	2.7e-03	-0.015750	102
C1	H16	3.828140	0.092400	0.093076	2.7e-03	-0.015750	102
C8	C13	3.889290	0.066000	0.074692	1.5e-03	-0.011850	103
C7	C12	3.889290	0.066000	0.074692	1.5e-03	-0.011850	103
C3	H18	3.906167	0.093300	0.093982	2.7e-03	-0.015150	102
C4	H19	3.906167	0.093300	0.093982	2.7e-03	-0.015150	102
C2	H14	3.945358	0.093400	0.094083	2.7e-03	-0.017200	102
C2	H15	3.945358	0.093400	0.094083	2.7e-03	-0.017200	102
C3	C8	4.143270	0.062900	0.071184	1.4e-03	-0.011700	103
C4	C7	4.143270	0.062900	0.071184	1.4e-03	-0.011700	103
C8	H18	4.200913	0.128000	0.128936	3.7e-03	-0.016150	102
C7	H19	4.200913	0.128000	0.128936	3.7e-03	-0.016150	102
C6	C9	4.277546	0.065100	0.073674	1.5e-03	-0.014100	103
C5	C10	4.277546	0.065100	0.073674	1.5e-03	-0.014100	103
H19	H15	4.327662	0.130600	0.131555	3.8e-03	-0.021600	102
H14	H18	4.327662	0.130600	0.131555	3.8e-03	-0.021600	102
C7	H22	4.326235	0.142100	0.143139	4.1e-03	-0.017350	102
C8	H23	4.326235	0.142100	0.143139	4.1e-03	-0.017350	102
C8	H21	4.326235	0.142100	0.143139	4.1e-03	-0.017350	102
C7	H20	4.326235	0.142100	0.143139	4.1e-03	-0.017350	102
C10	C13	4.311622	0.066750	0.075541	1.5e-03	-0.007350	103
C9	C12	4.311622	0.066750	0.075541	1.5e-03	-0.007350	103
C13	H14	4.352410	0.123300	0.124201	3.6e-03	0.002700	102
C12	H15	4.352410	0.123300	0.124201	3.6e-03	0.002700	102
C2	H22	4.409694	0.189500	0.190885	5.5e-03	0.010800	102
C2	H23	4.409694	0.189500	0.190885	5.5e-03	0.010800	102
C2	H21	4.409694	0.189500	0.190885	5.5e-03	0.010800	102
C2	H20	4.409694	0.189500	0.190885	5.5e-03	0.010800	102
C4	H14	4.481011	0.103500	0.104257	3.0e-03	-0.014000	102
C3	H15	4.481011	0.103500	0.104257	3.0e-03	-0.014000	102
C5	H23	4.465334	0.219900	0.221508	6.3e-03	0.028000	102
C6	H22	4.465334	0.219900	0.221508	6.3e-03	0.028000	102
C6	H20	4.465334	0.219900	0.221508	6.3e-03	0.028000	102
C5	H21	4.465334	0.219900	0.221508	6.3e-03	0.028000	102
C4	H18	4.637863	0.102800	0.103552	3.0e-03	-0.015400	102
C3	H19	4.637863	0.102800	0.103552	3.0e-03	-0.015400	102
C10	H16	4.690203	0.105000	0.105768	3.0e-03	-0.018700	102
C9	H17	4.690203	0.105000	0.105768	3.0e-03	-0.018700	102
C9	C13	4.744556	0.065400	0.074013	1.5e-03	-0.000200	103
C10	C12	4.744556	0.065400	0.074013	1.5e-03	-0.000200	103
C8	C12	4.750762	0.067000	0.075824	1.5e-03	0.002600	103
C7	C13	4.750762	0.067000	0.075824	1.5e-03	0.002600	103
C5	C6	4.772325	0.061300	0.069373	1.4e-03	-0.012300	103

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Table S13 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C13	H17	4.793552	0.106500	0.107279	3.1e-03	-0.018200	102
C12	H16	4.793552	0.106500	0.107279	3.1e-03	-0.018200	102
C7	C8	4.860961	0.063700	0.072089	1.4e-03	-0.014900	103
C9	H22	4.877711	0.167500	0.168725	4.8e-03	-0.003050	102
C10	H23	4.877711	0.167500	0.168725	4.8e-03	-0.003050	102
C9	H20	4.877711	0.167500	0.168725	4.8e-03	-0.003050	102
C10	H21	4.877711	0.167500	0.168725	4.8e-03	-0.003050	102
H16	H19	4.931804	0.163600	0.164796	4.7e-03	-0.019800	102
H18	H17	4.931804	0.163600	0.164796	4.7e-03	-0.019800	102
C6	H18	4.966565	0.118300	0.119165	3.4e-03	-0.017300	102
C5	H19	4.966565	0.118300	0.119165	3.4e-03	-0.017300	102
C5	C8	5.025204	0.065200	0.073787	1.5e-03	-0.014000	103
C6	C7	5.025204	0.065200	0.073787	1.5e-03	-0.014000	103
H15	H20	4.971045	0.245000	0.246791	7.1e-03	0.027200	102
H15	H22	4.971045	0.245000	0.246791	7.1e-03	0.027200	102
H14	H21	4.971045	0.245000	0.246791	7.1e-03	0.027200	102
H14	H23	4.971045	0.245000	0.246791	7.1e-03	0.027200	102
H17	H23	5.132351	0.171800	0.173056	5.0e-03	-0.025800	102
H17	H21	5.132351	0.171800	0.173056	5.0e-03	-0.025800	102
H16	H20	5.132351	0.171800	0.173056	5.0e-03	-0.025800	102
H16	H22	5.132351	0.171800	0.173056	5.0e-03	-0.025800	102
C4	H16	5.227922	0.094900	0.095594	2.7e-03	-0.016500	102
C3	H17	5.227922	0.094900	0.095594	2.7e-03	-0.016500	102
C9	H15	5.360059	0.096500	0.097206	2.8e-03	-0.018250	102
C10	H14	5.360059	0.096500	0.097206	2.8e-03	-0.018250	102
C12	H18	5.392766	0.097600	0.098314	2.8e-03	-0.011350	102
C13	H19	5.392766	0.097600	0.098314	2.8e-03	-0.011350	102
C10	H20	5.436495	0.222350	0.223976	6.4e-03	0.020000	102
C9	H21	5.436495	0.222350	0.223976	6.4e-03	0.020000	102
C10	H22	5.436495	0.222350	0.223976	6.4e-03	0.020000	102
C9	H23	5.436495	0.222350	0.223976	6.4e-03	0.020000	102
C7	H21	5.447524	0.236050	0.237776	6.8e-03	0.027700	102
C8	H20	5.447524	0.236050	0.237776	6.8e-03	0.027700	102
C7	H23	5.447524	0.236050	0.237776	6.8e-03	0.027700	102
C8	H22	5.447524	0.236050	0.237776	6.8e-03	0.027700	102
C6	H14	5.722716	0.101800	0.102544	2.9e-03	-0.014300	102
C5	H15	5.722716	0.101800	0.102544	2.9e-03	-0.014300	102
C13	H18	5.759684	0.100500	0.101235	2.9e-03	-0.004200	102
C12	H19	5.759684	0.100500	0.101235	2.9e-03	-0.004200	102
C13	H16	5.777233	0.101400	0.102141	2.9e-03	-0.000400	102
C12	H17	5.777233	0.101400	0.102141	2.9e-03	-0.000400	102
C8	H16	5.849649	0.101700	0.102444	2.9e-03	-0.019000	102
C7	H17	5.849649	0.101700	0.102444	2.9e-03	-0.019000	102
H18	H20	5.943653	0.191450	0.192850	5.5e-03	-0.005125	102
H18	H22	5.943653	0.191450	0.192850	5.5e-03	-0.005125	102
H19	H21	5.943653	0.191450	0.192850	5.5e-03	-0.005125	102
H19	H23	5.943653	0.191450	0.192850	5.5e-03	-0.005125	102
H14	H19	6.034842	0.140400	0.141426	4.1e-03	-0.020600	102
H18	H15	6.034842	0.140400	0.141426	4.1e-03	-0.020600	102

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Table S13 – continued from previous page

Atom 1	Atom 2	r_a	$l_{calc.}$	$l_{exp.}$	σ_{MC}	$(r_e - r_a)$	Group
C8	H14	6.076772	0.098650	0.099371	2.8e-03	-0.016700	102
C7	H15	6.076772	0.098650	0.099371	2.8e-03	-0.016700	102
C5	H17	6.095710	0.097900	0.098616	2.8e-03	-0.018000	102
C6	H16	6.095710	0.097900	0.098616	2.8e-03	-0.018000	102
H18	H21	6.430083	0.240750	0.242510	7.0e-03	0.016200	102
H19	H20	6.430083	0.240750	0.242510	7.0e-03	0.016200	102
H19	H22	6.430083	0.240750	0.242510	7.0e-03	0.016200	102
H18	H23	6.430083	0.240750	0.242510	7.0e-03	0.016200	102
H17	H20	6.455666	0.260375	0.262279	7.5e-03	0.027300	102
H17	H22	6.455666	0.260375	0.262279	7.5e-03	0.027300	102
H16	H21	6.455666	0.260375	0.262279	7.5e-03	0.027300	102
H16	H23	6.455666	0.260375	0.262279	7.5e-03	0.027300	102
H14	H15	6.615957	0.135600	0.136591	3.9e-03	-0.014500	102
H16	H17	6.796193	0.133000	0.133972	3.8e-03	-0.022000	102
H16	H15	7.152067	0.122350	0.123244	3.5e-03	-0.019400	102
H14	H17	7.152067	0.122350	0.123244	3.5e-03	-0.019400	102

References

[1] Leena Sinha, Onkar Prasad, Vijay Narayan, and Rajesh K. Srivastava. Electronic structure, non-linear properties and vibrational analysis of acenaphthene and its carbonyl derivative acenaphthenequinone by density functional theory. *Journal of Molecular Structure: THEOCHEM*, 958(1):33 – 40, 2010.

[2] Sébastien Gruet, Amanda L. Steber, and Melanie Schnell. Reconnaissance of the uncharted low energy vibrational motions of acenaphthene. *Journal of Molecular Spectroscopy*, 371:111296, 2020.

[3] NIST Chemistry WebBook, URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=C83329&Mask=200#Mass-Spec (accessed Th Oct 06 2021).

[4] Tomáš Baše, Josef Holub, Jindřich Fanfrlík, Drahomír Hnyk, Paul D. Lane, Derek A. Wann, Yury V. Vishnevskiy, Denis Tikhonov, Christian G. Reuter, and Norbert W. Mitzel. Icosahedral carbaboranes with peripheral hydrogen–chalcogenide groups: Structures from gas electron diffraction and chemical shielding in solution. *Chemistry – A European Journal*, 25(9):2313–2321, 2019.

[5] Jette Oddershede and Sine Larsen. Charge density study of naphthalene based on x-ray diffraction data at four different temperatures and theoretical calculations. *The Journal of Physical Chemistry A*, 108(6):1057–1063, 2004.