ORGANOMETALLICS

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BAZAN
2126-2130

L-2130-M1

Supplementary Material for

Permethylcyclopentadienyl-Carbollide Derivatives of Scandium.

Experimental. Crystal an irregular chunk, 0.14×0.44×0.52 mm; CAD-4 diffractometer, ω scans; 25 reflections with 13° < 2θ <18° used for cell dimensions; empirical absorption correction based on psi scans, relative transmission from 0.908 to 1.104; $(\sin\theta/\lambda)_{max}$ = 0.59 Å^{-1}; h from −46 to 46, k from −13 to 13, l from 0 to 16; three standard reflections (152; 17,$\bar{1}$,$\bar{3}$; $\bar{8}2\bar{4}$)) showed a significant (~ 11%) decay, corrected by a quadratic function; 11087 reflections measured, 5130 independent. Goodness of fit for merging, 0.977 (R_{merge} for 2887 reflections with exactly two observations, 0.072); all reflections used in solution and refinement of the structure; scandium atom coordinates obtained from Patterson map, remaining heavy atoms found by successive structure factor–Fourier calculations; F_o^2 values (positive and negative) used in least squares calculations, with weights = $1/(\sigma^2(F_o^2)$; hydrogen atoms places at calculated positions (B–H, C–H = 0.95 Å) and not refined, but atoms repositioned once near end of refinement; coordinates of non-hydrogen atoms of the anion, the Li atoms and the two THF molecules, with anisotropic displacement parameters for the Sc atoms, C atoms of the Cp groups and atoms of the THF molecules, plus isotropic displacement parameters for the non-solvent heavy atoms refined; R (on F) for 4328 reflections with $F_o^2 > 0$ = 0.164, for 2148 reflections with $F_o^2 > 3\sigma(F_o^2)$ = 0.090, wR (on F^2) 0.031 for 4328 reflections and 0.026 for 2148 reflections, goodness of fit = 2.22. Weights taken as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data by propagation of error plus another additional term, $(0.014\bar{I})^2$; maximum shift/esd 0.10 except for the THF atoms, where maximum is 0.71; final difference map shows peaks of +1.24 eÅ^{-3} and valleys of −0.99 eÅ^{-3}; no correction for secondary extinction; atomic scattering factors and values for $\Delta f'$ taken from Cromer and Waber (1974) and Cromer (1974); programs used were those of the CRYM Crystallographic Computing System (Duchamp, 1964) and ORTEP (Johnson, 1976). Final parameters are given in Table 1 with complete distances and angles

in Table 2. Anisotropic displacement parameters are listed in Table 3, assigned hydrogen parameters and solvent parameters in Table 4, with structure factors in Table 5.

The crystal includes disordered toluene solvent at three locations in the unit cell, one at a center of symmetry and two on two-fold axes. These regions were modeled with an idealized toluene molecule placed in each one based on a Fourier map; the molecules were moved twice to improve the appearance of a difference map. After final refinement in C2/c (the toluene parameters not being refined) the structure was re-cast in Cc, with eight possibilities for the 3 solvent regions, and structure factors calculated. None of the eight was significantly better than the rest; the best gave (compared to the C2/c refinement results in brackets) R = 0.161 [0.166], R(on F, for $F_o^2 > 3\sigma(F_o^2)$=0.089 [0.090], goodness of fit 2.11 [2.24]. That best model was refined by least squares, but the refinement diverged in the first cycle; the structure is so nearly centrosymmetric that the small departures from centrosymmetry in the solvent regions were insignificant. Therefore we report the result of the refinement in C2/c, even though we recognize that the disorder in the solvent regions is at best a rough approximation of the true structure. In addition, the tetrahydrofuran molecules coordinated to the Li atom are poorly defined and one – C8 – has a ridiculous anisotropic displacement parameter, corresponding to a mean displacement of 1.1 Å! Finally, although we expected a second Li atom for charge balance, it is nowhere to be found, unless one of the three solvent regions that we modelled with toluene really conceals a Li atom and coordinated THF. The difference maps do not suggest this, but we could probably fit any of the three regions with an $Li(THF)_2^+$ group about as well as we did with the toluene molecules.

L-2130-M3

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G., Taylor, R. (1987) *J. Chem. Soc. Perkin Trans.* S1–S19.

Cromer, D. T., (1974) *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151.

Cromer, D. T. & Waber, J. T. (1974) *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101.

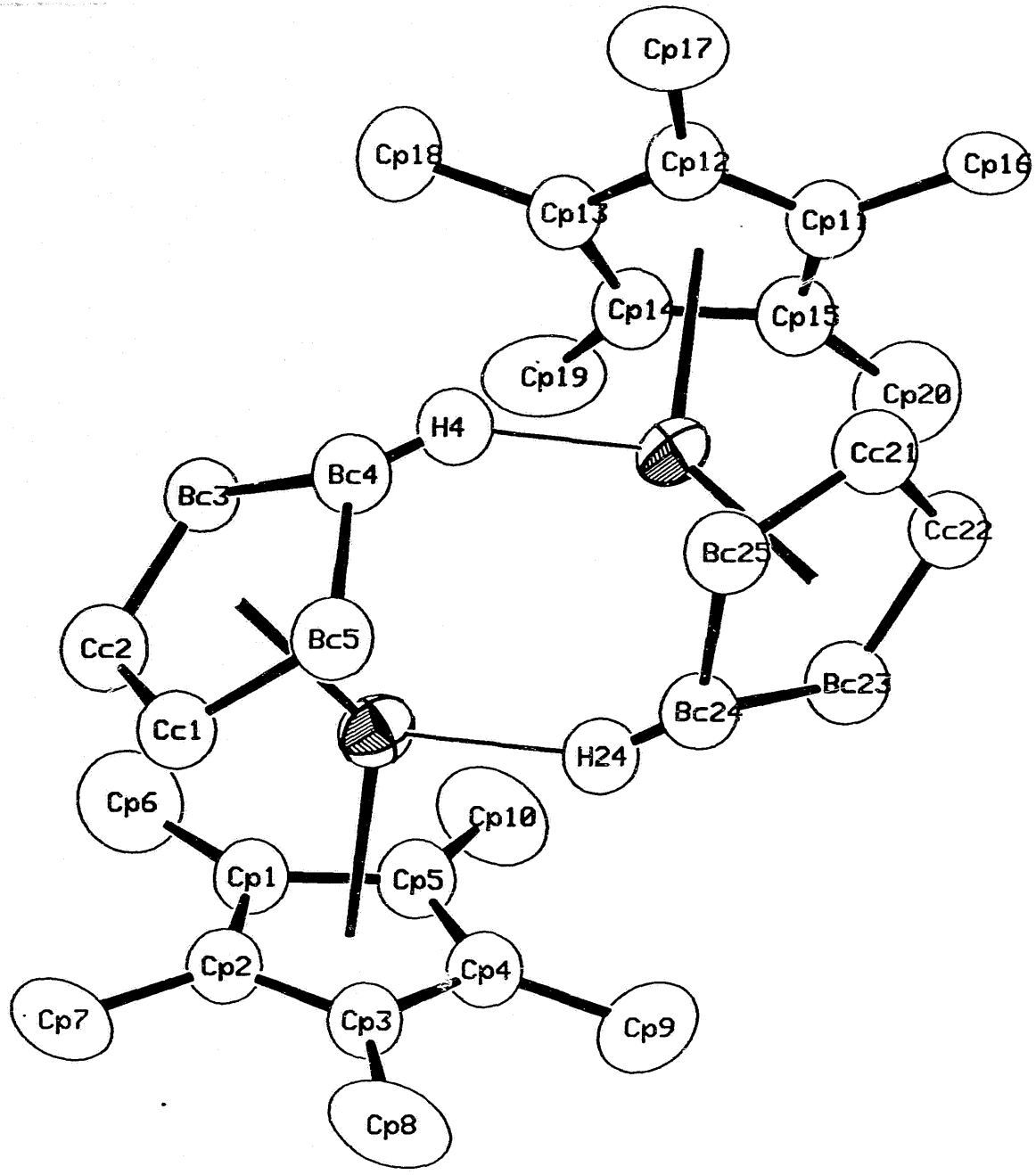
Duchamp. D. J. (1964) A.C.A. Meeting, Bozeman, Montana, paper B-14, p. 29.

Johnson, C. K. (1976) ORTEP-II, A FORTRAN Thermal Ellipsoid Plot Program for Crystal Structure Illustrations. Report ORNL-3794, Third Revision, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Larson, A. C., (1967) *Acta Crystallog.*, *23*, 644, eqn 3.

Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989) *J. Chem. Soc. Dalton Trans.* S1–S38.

Figure 1. An ORTEP drawing of a portion of the cation with 50% probability ellipsoids showing the numbering system. Of the hydrogen atoms, only H4 and H24 are shown. Hydrogen atoms are not shown.



AW-031E-7

L-2130-M5

Table S1. Non-Refined Parameters for Cp*, Dicarbollide Scandium Dimer.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	B	
H6 A	900	−697	240	6.6	*
H6 B	1102	−1591	454	6.6	*
H6 C	1229	−587	352	6.6	*
H7 A	470	−303	1542	4.6	*
H7 B	532	−1401	1559	4.6	*
H7 C	545	−786	808	4.6	*
H8 A	998	−73	3796	6.2	*
H8 B	802	−945	3424	6.2	*
H8 C	714	86	3088	6.2	*
H9 A	1742	−231	3712	5.6	*
H9 B	1653	−1304	3731	5.6	*
H9 C	1504	−519	4111	5.6	*
H10A	1701	−708	1422	5.0	*
H10B	1740	−1562	2036	5.0	*
H10C	1849	−539	2354	5.0	*
H16A	2428	836	7292	4.8	*
H16B	2667	573	6887	4.8	*
H16C	2472	1472	6588	4.8	*
H17A	3319	257	8563	6.2	*
H17B	3028	−89	7959	6.2	*
H17C	3060	11	8891	6.2	*
H18A	3461	2570	9909	5.5	*
H18B	3497	1492	9713	5.5	*
H18C	3261	1799	10117	5.5	*
H19A	3207	4103	9138	6.9	*
H19B	2958	3821	9500	6.9	*
H19C	2888	4358	8664	6.9	*
H20A	2553	4019	7555	5.9	*
H20B	2336	3164	7388	5.9	*
H20C	2505	3402	6765	5.9	*
H1	600	1220	1897	4.2	*

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Table S1. (Cont.)

Atom	x	y	z	B	
H2	720	690	580	4.2	*
H3	1170	1660	400	4.2	*
H4	1340	2920	1750	4.2	*
H5	950	2590	2670	4.2	*
H6	400	3050	1770	4.2	*
H7	240	1840	400	4.2	*
H8	620	2140	−550	4.2	*
H9	1010	3600	210	4.2	*
H10	890	4180	1650	4.2	*
H11	410	3600	220	4.2	*
H21	3080	850	6550	4.2	*
H22	2730	2300	6180	4.2	*
H23	3060	3910	6350	4.2	*
H24	3610	3430	6780	4.2	*
H25	3650	1390	6940	4.2	*
H26	3370	640	5380	4.2	*
H27	2790	1190	4950	4.2	*
H28	2770	3130	4780	4.2	*
H29	3340	3950	5150	4.2	*
H30	3720	2270	5540	4.2	*
H31	3180	2180	4280	4.2	*
Cs1	2548	3917	816	10.0	*
Cs2	2548	3043	438	10.0	*
Cs3	2723	2318	851	10.0	*
Cs4	2721	1422	451	10.0	*
Cs5	2545	1286	−340	10.0	*
Cs6	2369	2023	−752	10.0	*
Cs7	2367	2919	−371	10.0	*
Cs11	5105	319	1494	14.0	*
Cs12	5036	629	2153	14.0	*
Cs13	5022	1622	2292	14.0	*

L-2130-M7

Table S1. (Cont.)

Atom	x	y	z	B	
Cs14	4947	1933	3004	14.0	*
Cs15	4890	1287	3542	14.0	*
Cs16	4905	307	3403	14.0	*
Cs17	4978	−28	2709	14.0	*
Cs21	−219	−119	978	14.0	*
Cs22	−105	156	1770	14.0	*
Cs23	−17	−538	2378	14.0	*
Cs24	103	−263	3210	14.0	*
Cs25	129	706	3393	14.0	*
Cs26	41	1400	2784	14.0	*
Cs27	−76	1125	1972	14.0	*
Hs1	2416	4338	453	12.0	*
Hs8	2491	3829	1298	12.0	*
Hs9	2736	4185	959	12.0	*
Hs41	2679	3896	1354	12.0	*
Hs48	2359	4050	848	12.0	*
Hs49	2605	4406	509	12.0	*
Hs3	2844	2413	1395	12.0	*
Hs4	2841	914	729	12.0	*
Hs5	2545	685	−603	12.0	*
Hs6	2249	1923	−1296	12.0	*
Hs7	2247	3426	−651	12.0	*
Hs11	5106	−364	1489	16.0	*
Hs18	4968	549	1011	16.0	*
Hs19	5291	549	1513	16.0	*
Hs51	5137	853	1186	16.0	*
Hs58	4952	−59	1162	16.0	*
Hs59	5276	−59	1664	16.0	*
Hs13	5060	2075	1922	16.0	*
Hs14	4936	2601	3105	16.0	*
Hs15	4841	1509	4010	16.0	*

L-2130-M8

Table S1. (Cont.)

Atom	x	y	z	B	
Hs16	4866	−140	3778	16.0	*
Hs17	4987	−699	2617	16.0	*
Hs21	−267	433	639	16.0	*
Hs28	−81	−492	814	16.0	*
Hs29	−387	−492	927	16.0	*
Hs61	−223	−800	947	16.0	*
Hs68	−103	125	660	16.0	*
Hs69	−409	125	773	16.0	*
Hs23	−38	−1199	2237	16.0	*
Hs24	163	−732	3630	16.0	*
Hs25	209	902	3947	16.0	*
Hs26	61	2061	2924	16.0	*
Hs27	−135	1598	1556	16.0	*
Hf1a	3720	1800	2832	15.6	*
Hf1b	3607	2218	1953	15.6	*
Hf2a	4026	2523	2023	15.6	*
Hf2b	4136	1943	2832	15.6	*
Hf3a	4254	771	2112	15.6	*
Hf3b	4090	1258	1289	15.6	*
Hf4a	3483	1013	1728	15.6	*
Hf4b	3648	671	2607	15.6	*
Hf5a	4346	2462	5852	17.2	*
Hf5b	4595	1856	6411	17.2	*
Hf6a	4643	1053	5441	17.2	*
Hf6b	4574	2061	5045	17.2	*
Hf7a	4300	832	4336	17.2	*
Hf7b	4129	1703	4516	17.2	*
Hf8a	4214	−11	5252	17.2	*
Hf8b	3936	607	5011	17.2	*

L-2130-M9

Table S2. Anisotropic Displacement Parameters for Cp*, Dicarbollide Scandium Dimer.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sc1	488(17)	408(16)	355(16)	31(15)	153(13)	−7(16)
Cp6	828(111)	815(112)	900(121)	−65(97)	288(94)	−127(108)
Cp7	697(106)	666(102)	749(109)	−155(85)	287(87)	−29(90)
Cp8	967(120)	783(116)	981(126)	−245(92)	584(104)	−147(99)
Cp9	1092(125)	503(100)	715(113)	30(88)	89(99)	156(86)
Cp10	591(96)	581(97)	1104(124)	8(84)	393(89)	−64(95)
Sc2	473(16)	505(16)	302(14)	−46(16)	116(12)	39(16)
Cp16	710(98)	627(99)	458(92)	−283(85)	191(79)	78(85)
Cp17	892(116)	834(123)	964(127)	−46(95)	498(100)	200(104)
Cp18	605(99)	1433(144)	458(98)	−284(92)	164(83)	113(95)
Cp19	1441(139)	656(109)	671(108)	−224(103)	639(100)	−122(95)
Cp20	756(111)	863(117)	785(120)	130(92)	285(93)	69(96)
O1	2346(191)	864(115)	1994(149)	−941(127)	1325(137)	−502(102)
C1	3388(541)	962(279)	2750(408)	780(358)	538(377)	−425(268)
C2	3509(638)	1421(347)	4259(639)	−719(444)	1591(483)	−937(345)
C3	2873(348)	1451(259)	1173(189)	−446(290)	881(201)	21(200)
C4	1673(226)	1233(248)	1641(219)	489(183)	557(168)	13(175)
O2	2945(219)	2040(225)	3678(276)	1467(200)	3075(228)	1221(215)
C5	1845(275)	2198(323)	2353(361)	−180(220)	783(247)	77(271)
C6	2591(350)	4208(485)	1445(279)	38(287)	1752(287)	−380(270)
C7	3876(496)	1384(243)	1237(250)	273(260)	−126(276)	−657(187)
C8	6340(684)	1108(263)	9585(999)	−1043(331)	7649(775)	−1262(401)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S3. Distances and Angles for Cp*, Dicarbollide Scandium Dimer.

	Distance(Å)		Distance(Å)
Sc1 –Cp*1	2.206	Cp6 –H6 C	0.987
Sc1 –Cp1	2.525(12)	Cp7 –H7 A	0.905
Sc1 –Cp2	2.502(12)	Cp7 –H7 B	1.004
Sc1 –Cp3	2.490(12)	Cp7 –H7 C	1.009
Sc1 –Cp4	2.523(12)	Cp8 –H8 A	0.913
Sc1 –Cp5	2.505(12)	Cp8 –H8 B	1.004
Sc1 –Cb 1	2.082	Cp8 –H8 C	1.018
Sc1 –Cc1	2.514(12)	Cp9 –H9 A	1.027
Sc1 –Cc2	2.509(12)	Cp9 –H9 B	1.010
Sc1 –Bc3	2.501(14)	Cp9 –H9 C	0.923
Sc1 –Bc4	2.536(14)	Cp10 –H10A	0.995
Sc1 –Bc5	2.521(14)	Cp10 –H10B	0.944
Sc1 –H24	2.196	Cp10 –H10C	1.008
Sc2 –Cp*2	2.182	Cc1 –Cc2	1.567(16)
Sc2 –Cp11	2.493(13)	Cc1 –Bc5	1.626(18)
Sc2 –Cp12	2.484(13)	Cc1 –Bc6	1.731(19)
Sc2 –Cp13	2.517(12)	Cc1 –Bc7	1.724(19)
Sc2 –Cp14	2.486(12)	Cc1 –H1	0.975
Sc2 –Cp15	2.467(12)	Cc2 –Bc3	1.608(18)
Sc2 –Cb 2	2.081	Cc2 –Bc7	1.73(2)
Sc2 –Cc21	2.484(13)	Cc2 –Bc8	1.689(19)
Sc2 –Cc22	2.495(11)	Cc2 –H2	0.974
Sc2 –Bc23	2.488(13)	Bc3 –Bc4	1.737(19)
Sc2 –Bc24	2.554(14)	Bc3 –Bc8	1.76(2)
Sc2 –Bc25	2.536(15)	Bc3 –Bc9	1.81(2)
Sc2 –H4	2.173	Bc3 –H3	0.964
Cp1 –Cp2	1.438(17)	Bc4 –Bc5	1.77(2)
Cp1 –Cp5	1.430(17)	Bc4 –Bc9	1.76(2)
Cp1 –Cp6	1.470(18)	Bc4 –Bc10	1.80(2)
Cp2 –Cp3	1.367(17)	Bc4 –H4	1.001
Cp2 –Cp7	1.541(17)	Bc5 –Bc6	1.77(2)
Cp3 –Cp4	1.417(17)	Bc5 –Bc10	1.76(2)
Cp3 –Cp8	1.494(18)	Bc5 –H5	0.965
Cp4 –Cp5	1.379(17)	Bc6 –Bc7	1.75(2)
Cp4 –Cp9	1.498(18)	Bc6 –Bc10	1.69(2)
Cp5 –Cp10	1.494(17)	Bc6 –Bc11	1.71(2)
Cp6 –H6 A	0.966	Bc6 –H6	1.040
Cp6 –H6 B	0.982	Bc7 –Bc8	1.77(2)

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Table S3. (Cont.)

	Distance(Å)		Distance(Å)
Bc7 –Bc11	1.68(2)	Cc21 –Bc26	1.75(2)
Bc7 –H7	1.025	Cc21 –Bc27	1.77(2)
Bc8 –Bc9	1.74(2)	Cc21 –H21	0.997
Bc8 –Bc11	1.75(2)	Cc22 –Bc23	1.612(17)
Bc8 –H8	1.012	Cc22 –Bc27	1.721(19)
Bc9 –Bc10	1.77(2)	Cc22 –Bc28	1.695(18)
Bc9 –Bc11	1.76(2)	Cc22 –H22	1.030
Bc9 –H9	1.028	Bc23 –Bc24	1.705(19)
Bc10 –Bc11	1.79(2)	Bc23 –Bc28	1.77(2)
Bc10 –H10	1.038	Bc23 –Bc29	1.759(19)
Bc11 –H11	0.981	Bc23 –H23	0.922
Cp11 –Cp12	1.401(17)	Bc24 –Bc25	1.72(2)
Cp11 –Cp15	1.386(17)	Bc24 –Bc29	1.80(2)
Cp11 –Cp16	1.505(17)	Bc24 –Bc30	1.74(2)
Cp12 –Cp13	1.415(17)	Bc24 –H24	0.971
Cp12 –Cp17	1.495(18)	Bc25 –Bc26	1.80(2)
Cp13 –Cp14	1.419(17)	Bc25 –Bc30	1.75(2)
Cp13 –Cp18	1.510(17)	Bc25 –H25	1.086
Cp14 –Cp15	1.411(17)	Bc26 –Bc27	1.75(2)
Cp14 –Cp19	1.497(18)	Bc26 –Bc30	1.81(2)
Cp15 –Cp20	1.457(18)	Bc26 –Bc31	1.75(2)
Cp16 –H16A	0.915	Bc26 –H26	0.997
Cp16 –H16B	1.004	Bc27 –Bc28	1.76(2)
Cp16 –H16C	0.983	Bc27 –Bc31	1.75(2)
Cp17 –H17A	0.956	Bc27 –H27	0.973
Cp17 –H17B	0.968	Bc28 –Bc29	1.73(2)
Cp17 –H17C	0.992	Bc28 –Bc31	1.75(2)
Cp18 –H18A	0.968	Bc28 –H28	0.933
Cp18 –H18B	0.985	Bc29 –Bc30	1.84(2)
Cp18 –H18C	1.005	Bc29 –Bc31	1.77(2)
Cp19 –H19A	0.970	Bc29 –H29	1.037
Cp19 –H19B	0.991	Bc30 –Bc31	1.83(2)
Cp19 –H19C	0.955	Bc30 –H30	0.999
Cp20 –H20A	1.000	Bc31 –H31	0.976
Cp20 –H20B	1.047	O1 –C3	1.36(4)
Cp20 –H20C	0.945	O1 –C4	1.39(3)
Cc21 –Cc22	1.586(17)	O1 –Li1	1.85(5)
Cc21 –Bc25	1.65(2)	C1 –C2	1.33(7)

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Table S3. (Cont.)

	Distance(Å)		Distance(Å)
C1 –C4	1.54(5)	Cs5 –Hs5	0.950
C1 –Hf1a	0.823	Cs6 –Cs7	1.409
C1 –Hf1b	1.034	Cs6 –Hs6	0.950
C2 –C3	1.38(6)	Cs7 –Hs7	0.950
C2 –Hf2a	0.884	Cs11 –Cs12	1.338
C2 –Hf2b	1.206	Cs11 –Hs11	0.950
C3 –Hf3a	0.908	Cs11 –Hs18	0.950
C3 –Hf3b	0.962	Cs11 –Hs19	0.950
C4 –Hf4a	0.947	Cs11 –Hs51	0.950
C4 –Hf4b	0.938	Cs11 –Hs58	0.950
O2 –C5	1.54(4)	Cs11 –Hs59	0.950
O2 –C8	0.96(6)	Cs12 –Cs13	1.408
C5 –C6	1.40(5)	Cs12 –Cs17	1.406
C5 –C8	1.85(6)	Cs12 –Hs11	1.882
C5 –Hf5a	1.062	Cs12 –Hs18	1.882
C5 –Hf5b	0.914	Cs12 –Hs19	1.882
C6 –C7	1.39(5)	Cs12 –Hs51	1.882
C6 –Hf6a	0.998	Cs12 –Hs58	1.882
C6 –Hf6b	0.894	Cs12 –Hs59	1.882
C7 –C8	1.44(6)	Cs13 –Cs14	1.433
C7 –Hf7a	0.920	Cs13 –Hs13	0.950
C7 –Hf7b	1.005	Cs14 –Cs15	1.370
C8 –Hf8a	1.066	Cs14 –Hs14	0.950
C8 –Hf8b	1.381	Cs15 –Cs16	1.392
Cs1 –Cs2	1.378	Cs15 –Hs15	0.950
Cs1 –Hs1	0.950	Cs16 –Cs17	1.412
Cs1 –Hs8	0.950	Cs16 –Hs16	0.950
Cs1 –Hs9	0.950	Cs17 –Hs17	0.950
Cs1 –Hs41	0.950	Cs21 –Cs22	1.355
Cs1 –Hs48	0.950	Cs21 –Hs21	0.950
Cs1 –Hs49	0.950	Cs21 –Hs28	0.950
Cs2 –Cs3	1.375	Cs21 –Hs29	0.950
Cs2 –Cs7	1.412	Cs21 –Hs61	0.950
Cs3 –Cs4	1.421	Cs21 –Hs68	0.950
Cs3 –Hs3	0.950	Cs21 –Hs69	0.950
Cs4 –Cs5	1.381	Cs22 –Cs23	1.390
Cs4 –Hs4	0.950	Cs22 –Cs27	1.390
Cs5 –Cs6	1.388	Cs23 –Cs24	1.419

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Table S3. (Cont.)

Distance(Å)		Angle(°)	
Cs23 –Hs23	0.950	Cb 1 –Sc1 –Cp*1	136.3
Cs24 –Cs25	1.382	H24 –Sc1 –Cp*1	105.6
Cs24 –Hs24	0.950	H24 –Sc1 –Cb 1	107.6
Cs25 –Cs23	1.390	Bc24 –H24 –Sc1	148.8
Cs25 –Hs25	0.950	Cb 2 –Sc2 –Cp*2	136.5
Cs26 –Cs27	1.387	H4 –Sc2 –Cb 2	106.7
Cs26 –Hs26	0.950	H4 –Sc2 –Cp*2	107.4
Cs27 –Hs27	0.950	Bc4 –H4 –Sc2	145.4
		Cp5 –Cp1 –Cp2	106.0(10)
		Cp6 –Cp1 –Cp2	125.4(11)
		Cp6 –Cp1 –Cp5	128.6(11)
		Cp3 –Cp2 –Cp1	108.3(10)
		Cp7 –Cp2 –Cp1	124.6(10)
		Cp7 –Cp2 –Cp3	126.2(11)
		Cp4 –Cp3 –Cp2	109.1(11)
		Cp8 –Cp3 –Cp2	126.7(11)
		Cp8 –Cp3 –Cp4	124.1(11)
		Cp5 –Cp4 –Cp3	107.9(11)
		Cp9 –Cp4 –Cp3	126.8(11)
		Cp9 –Cp4 –Cp5	124.3(11)
		Cp4 –Cp5 –Cp1	108.7(11)
		Cp10 –Cp5 –Cp1	122.9(11)
		Cp10 –Cp5 –Cp4	127.4(11)
		Bc5 –Cc1 –Cc2	111.7(9)
		Bc6 –Cc1 –Cc2	111.1(9)
		Bc7 –Cc1 –Cc2	63.4(8)
		Bc6 –Cc1 –Bc5	63.6(8)
		Bc7 –Cc1 –Bc5	115.0(10)
		Bc7 –Cc1 –Bc6	60.9(8)
		Bc3 –Cc2 –Cc1	112.7(10)
		Bc7 –Cc2 –Cc1	62.7(8)
		Bc8 –Cc2 –Cc1	112.5(9)
		Bc7 –Cc2 –Bc3	116.2(10)
		Bc8 –Cc2 –Bc3	64.3(8)
		Bc8 –Cc2 –Bc7	62.2(8)
		Bc4 –Bc3 –Cc2	105.3(10)
		Bc8 –Bc3 –Cc2	60.1(8)
		Bc9 –Bc3 –Cc2	103.4(10)

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Table S3. (Cont.)

	Angle(°)		Angle(°)
Bc8 –Bc3 –Bc4	107.6(10)	Bc11 –Bc8 –Cc2	103.2(10)
Bc9 –Bc3 –Bc4	59.3(8)	Bc7 –Bc8 –Bc3	107.3(10)
Bc9 –Bc3 –Bc8	58.2(8)	Bc9 –Bc8 –Bc3	62.6(8)
Bc5 –Bc4 –Bc3	105.6(10)	Bc11 –Bc8 –Bc3	109.6(10)
Bc9 –Bc4 –Bc3	62.5(8)	Bc9 –Bc8 –Bc7	106.5(11)
Bc10 –Bc4 –Bc3	108.8(10)	Bc11 –Bc8 –Bc7	57.2(9)
Bc9 –Bc4 –Bc5	106.6(10)	Bc11 –Bc8 –Bc9	60.5(9)
Bc10 –Bc4 –Bc5	59.3(8)	Bc4 –Bc9 –Bc3	58.1(8)
Bc10 –Bc4 –Bc9	59.5(8)	Bc8 –Bc9 –Bc3	59.2(8)
Bc4 –Bc5 –Cc1	104.5(10)	Bc10 –Bc9 –Bc3	106.8(10)
Bc6 –Bc5 –Cc1	61.1(8)	Bc11 –Bc9 –Bc3	106.6(10)
Bc10 –Bc5 –Cc1	104.8(10)	Bc8 –Bc9 –Bc4	107.4(10)
Bc6 –Bc5 –Bc4	107.0(10)	Bc10 –Bc9 –Bc4	61.4(8)
Bc10 –Bc5 –Bc4	61.3(8)	Bc11 –Bc9 –Bc4	109.5(11)
Bc10 –Bc5 –Bc6	57.1(8)	Bc10 –Bc9 –Bc8	108.9(11)
Bc5 –Bc6 –Cc1	55.3(7)	Bc11 –Bc9 –Bc8	60.1(9)
Bc7 –Bc6 –Cc1	59.3(8)	Bc11 –Bc9 –Bc10	61.0(9)
Bc10 –Bc6 –Cc1	103.5(10)	Bc5 –Bc10 –Bc4	59.4(8)
Bc11 –Bc6 –Cc1	103.2(10)	Bc6 –Bc10 –Bc4	109.1(10)
Bc7 –Bc6 –Bc5	106.7(10)	Bc9 –Bc10 –Bc4	59.2(8)
Bc10 –Bc6 –Bc5	61.2(8)	Bc11 –Bc10 –Bc4	106.3(10)
Bc11 –Bc6 –Bc5	109.8(11)	Bc6 –Bc10 –Bc5	61.6(8)
Bc10 –Bc6 –Bc7	109.6(11)	Bc9 –Bc10 –Bc5	106.4(10)
Bc11 –Bc6 –Bc7	58.1(9)	Bc11 –Bc10 –Bc5	106.8(10)
Bc11 –Bc6 –Bc10	63.4(9)	Bc9 –Bc10 –Bc6	107.4(11)
Cc2 –Bc7 –Cc1	53.9(7)	Bc11 –Bc10 –Bc6	58.9(9)
Bc6 –Bc7 –Cc1	59.8(8)	Bc11 –Bc10 –Bc9	59.2(8)
Bc8 –Bc7 –Cc1	101.8(10)	Bc7 –Bc11 –Bc6	62.0(9)
Bc11 –Bc7 –Cc1	104.8(11)	Bc8 –Bc11 –Bc6	110.0(11)
Bc6 –Bc7 –Cc2	102.7(10)	Bc9 –Bc11 –Bc6	106.8(11)
Bc8 –Bc7 –Cc2	57.7(8)	Bc10 –Bc11 –Bc6	57.7(8)
Bc11 –Bc7 –Cc2	104.1(11)	Bc8 –Bc11 –Bc7	62.0(9)
Bc8 –Bc7 –Bc6	107.5(11)	Bc9 –Bc11 –Bc7	109.4(11)
Bc11 –Bc7 –Bc6	59.8(9)	Bc10 –Bc11 –Bc7	108.2(11)
Bc11 –Bc7 –Bc8	60.8(9)	Bc9 –Bc11 –Bc8	59.4(9)
Bc3 –Bc8 –Cc2	55.6(8)	Bc10 –Bc11 –Bc8	107.4(11)
Bc7 –Bc8 –Cc2	60.2(8)	Bc10 –Bc11 –Bc9	59.8(9)
Bc9 –Bc8 –Cc2	103.4(10)	Cp15 –Cp11 –Cp12	110.3(11)

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Table S3. (Cont.)

	Angle(°)		Angle(°)
Cp16 –Cp11 –Cp12	124.1(11)	Bc24 –Bc25 –Cc21	105.7(10)
Cp16 –Cp11 –Cp15	124.7(11)	Bc26 –Bc25 –Cc21	60.8(8)
Cp13 –Cp12 –Cp11	106.8(11)	Bc30 –Bc25 –Cc21	108.7(10)
Cp17 –Cp12 –Cp11	127.5(11)	Bc26 –Bc25 –Bc24	108.2(10)
Cp17 –Cp12 –Cp13	125.3(11)	Bc30 –Bc25 –Bc24	59.9(8)
Cp14 –Cp13 –Cp12	107.4(10)	Bc30 –Bc25 –Bc26	61.2(8)
Cp18 –Cp13 –Cp12	125.8(11)	Bc25 –Bc26 –Cc21	55.3(8)
Cp18 –Cp13 –Cp14	126.3(11)	Bc27 –Bc26 –Cc21	60.4(8)
Cp15 –Cp14 –Cp13	108.4(11)	Bc30 –Bc26 –Cc21	101.9(10)
Cp19 –Cp14 –Cp13	123.4(11)	Bc31 –Bc26 –Cc21	104.8(10)
Cp19 –Cp14 –Cp15	127.8(11)	Bc27 –Bc26 –Bc25	106.6(10)
Cp14 –Cp15 –Cp11	106.8(11)	Bc30 –Bc26 –Bc25	58.0(8)
Cp20 –Cp15 –Cp11	128.9(11)	Bc31 –Bc26 –Bc25	106.7(10)
Cp20 –Cp15 –Cp14	123.7(11)	Bc30 –Bc26 –Bc27	109.5(10)
Bc25 –Cc21 –Cc22	110.0(10)	Bc31 –Bc26 –Bc27	60.1(9)
Bc26 –Cc21 –Cc22	108.8(10)	Bc31 –Bc26 –Bc30	61.9(8)
Bc27 –Cc21 –Cc22	61.5(8)	Cc22 –Bc27 –Cc21	54.1(7)
Bc26 –Cc21 –Bc25	63.8(8)	Bc26 –Bc27 –Cc21	59.8(8)
Bc27 –Cc21 –Bc25	113.1(10)	Bc28 –Bc27 –Cc21	102.6(10)
Bc27 –Cc21 –Bc26	59.8(8)	Bc31 –Bc27 –Cc21	104.1(10)
Bc23 –Cc22 –Cc21	111.3(9)	Bc26 –Bc27 –Cc22	102.8(10)
Bc27 –Cc22 –Cc21	64.4(8)	Bc28 –Bc27 –Cc22	58.3(8)
Bc28 –Cc22 –Cc21	113.8(9)	Bc31 –Bc27 –Cc22	102.9(10)
Bc27 –Cc22 –Bc23	115.8(9)	Bc28 –Bc27 –Bc26	107.7(11)
Bc28 –Cc22 –Bc23	64.7(8)	Bc31 –Bc27 –Bc26	59.8(9)
Bc28 –Cc22 –Bc27	61.9(8)	Bc31 –Bc27 –Bc28	59.8(9)
Bc24 –Bc23 –Cc22	107.0(9)	Bc23 –Bc28 –Cc22	55.4(7)
Bc28 –Bc23 –Cc22	59.9(8)	Bc27 –Bc28 –Cc22	59.8(8)
Bc29 –Bc23 –Cc22	106.1(9)	Bc29 –Bc28 –Cc22	104.0(10)
Bc28 –Bc23 –Bc24	109.3(10)	Bc31 –Bc28 –Cc22	104.2(10)
Bc29 –Bc23 –Bc24	62.5(8)	Bc27 –Bc28 –Bc23	106.3(10)
Bc29 –Bc23 –Bc28	58.5(8)	Bc29 –Bc28 –Bc23	60.4(8)
Bc25 –Bc24 –Bc23	105.9(10)	Bc31 –Bc28 –Bc23	106.9(10)
Bc29 –Bc24 –Bc23	60.2(8)	Bc29 –Bc28 –Bc27	109.9(11)
Bc30 –Bc24 –Bc23	110.3(10)	Bc31 –Bc28 –Bc27	60.0(9)
Bc29 –Bc24 –Bc25	109.2(10)	Bc31 –Bc28 –Bc29	61.1(9)
Bc30 –Bc24 –Bc25	60.9(8)	Bc24 –Bc29 –Bc23	57.3(8)
Bc30 –Bc24 –Bc29	62.6(8)	Bc28 –Bc29 –Bc23	61.1(8)

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Table S3. (Cont.)

	Angle(°)		Angle(°)
Bc30 –Bc29 –Bc23	103.4(9)	H7 C –Cp7 –H7 A	108.9
Bc31 –Bc29 –Bc23	106.8(10)	H7 C –Cp7 –H7 B	101.5
Bc28 –Bc29 –Bc24	107.2(10)	H8 A –Cp8 –Cp3	116.8
Bc30 –Bc29 –Bc24	57.0(8)	H8 B –Cp8 –Cp3	111.9
Bc31 –Bc29 –Bc24	105.9(10)	H8 C –Cp8 –Cp3	109.8
Bc30 –Bc29 –Bc28	108.6(10)	H8 B –Cp8 –H8 A	108.7
Bc31 –Bc29 –Bc28	60.2(8)	H8 C –Cp8 –H8 A	107.6
Bc31 –Bc29 –Bc30	61.1(8)	H8 C –Cp8 –H8 B	100.9
Bc25 –Bc30 –Bc24	59.3(8)	H9 A –Cp9 –Cp4	112.0
Bc26 –Bc30 –Bc24	107.4(10)	H9 B –Cp9 –Cp4	112.3
Bc29 –Bc30 –Bc24	60.4(8)	H9 C –Cp9 –Cp4	117.8
Bc31 –Bc30 –Bc24	105.8(10)	H9 B –Cp9 –H9 A	99.8
Bc26 –Bc30 –Bc25	60.8(8)	H9 C –Cp9 –H9 A	106.0
Bc29 –Bc30 –Bc25	106.2(10)	H9 C –Cp9 –H9 B	107.3
Bc31 –Bc30 –Bc25	105.3(10)	H10A –Cp10 –Cp5	113.3
Bc29 –Bc30 –Bc26	104.2(9)	H10B –Cp10 –Cp5	115.7
Bc31 –Bc30 –Bc26	57.3(8)	H10C –Cp10 –Cp5	111.6
Bc31 –Bc30 –Bc29	57.6(8)	H10B –Cp10 –H10A	107.0
Bc27 –Bc31 –Bc26	60.1(9)	H10C –Cp10 –H10A	102.2
Bc28 –Bc31 –Bc26	108.3(11)	H10C –Cp10 –H10B	106.0
Bc29 –Bc31 –Bc26	110.0(11)	H1 –Cc1 –Cc2	123.2
Bc30 –Bc31 –Bc26	60.8(8)	H1 –Cc1 –Bc5	116.3
Bc28 –Bc31 –Bc27	60.2(9)	H1 –Cc1 –Bc6	116.3
Bc29 –Bc31 –Bc27	108.2(11)	H1 –Cc1 –Bc7	116.7
Bc30 –Bc31 –Bc27	108.6(10)	H2 –Cc2 –Cc1	120.1
Bc29 –Bc31 –Bc28	58.8(8)	H2 –Cc2 –Bc3	118.5
Bc30 –Bc31 –Bc28	107.7(10)	H2 –Cc2 –Bc7	114.5
Bc30 –Bc31 –Bc29	61.3(8)	H2 –Cc2 –Bc8	116.2
H6 A –Cp6 –Cp1	113.1	H3 –Bc3 –Cc2	127.4
H6 B –Cp6 –Cp1	112.6	H3 –Bc3 –Bc4	122.6
H6 C –Cp6 –Cp1	113.6	H3 –Bc3 –Bc8	116.7
H6 B –Cp6 –H6 A	106.3	H3 –Bc3 –Bc9	118.2
H6 C –Cp6 –H6 A	105.8	H4 –Bc4 –Bc3	124.1
H6 C –Cp6 –H6 B	104.7	H4 –Bc4 –Bc5	121.5
H7 A –Cp7 –Cp2	115.3	H4 –Bc4 –Bc9	121.8
H7 B –Cp7 –Cp2	109.5	H4 –Bc4 –Bc10	119.9
H7 C –Cp7 –Cp2	111.5	H5 –Bc5 –Cc1	126.5
H7 B –Cp7 –H7 A	109.3	H5 –Bc5 –Bc4	124.0

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Table S3. (Cont.)

			Angle(°)				Angle(°)
H5	–Bc5	–Bc6	116.4	H17A	–Cp17	–Cp12	111.1
H5	–Bc5	–Bc10	116.3	H17B	–Cp17	–Cp12	113.0
H6	–Bc6	–Cc1	122.0	H17C	–Cp17	–Cp12	112.1
H6	–Bc6	–Bc5	120.6	H17B	–Cp17	–H17A	108.5
H6	–Bc6	–Bc7	119.6	H17C	–Cp17	–H17A	106.4
H6	–Bc6	–Bc10	124.6	H17C	–Cp17	–H17B	105.3
H6	–Bc6	–Bc11	125.2	H18A	–Cp18	–Cp13	116.5
H7	–Bc7	–Cc1	126.7	H18B	–Cp18	–Cp13	113.8
H7	–Bc7	–Cc2	127.8	H18C	–Cp18	–Cp13	111.7
H7	–Bc7	–Bc6	121.4	H18B	–Cp18	–H18A	106.0
H7	–Bc7	–Bc8	122.9	H18C	–Cp18	–H18A	104.3
H7	–Bc7	–Bc11	121.0	H18C	–Cp18	–H18B	103.3
H8	–Bc8	–Cc2	127.5	H19A	–Cp19	–Cp14	112.9
H8	–Bc8	–Bc3	124.7	H19B	–Cp19	–Cp14	111.9
H8	–Bc8	–Bc7	119.4	H19C	–Cp19	–Cp14	111.6
H8	–Bc8	–Bc9	123.0	H19B	–Cp19	–H19A	105.4
H8	–Bc8	–Bc11	119.6	H19C	–Cp19	–H19A	108.2
H9	–Bc9	–Bc3	121.3	H19C	–Cp19	–H19B	106.4
H9	–Bc9	–Bc4	120.4	H20A	–Cp20	–Cp15	115.5
H9	–Bc9	–Bc8	121.1	H20B	–Cp20	–Cp15	111.4
H9	–Bc9	–Bc10	122.8	H20C	–Cp20	–Cp15	119.0
H9	Bc9	–Bc11	123.3	H20B	–Cp20	–H20A	99.2
H10	–Bc10	–Bc4	116.8	H20C	–Cp20	–H20A	106.4
H10	–Bc10	–Bc5	123.5	H20C	–Cp20	–H20B	102.9
H10	–Bc10	–Bc6	127.1	H21	–Cc21	–Cc22	122.2
H10	–Bc10	–Bc9	117.7	H21	–Cc21	–Bc25	120.1
H10	–Bc10	–Bc11	125.1	H21	–Cc21	–Bc26	117.7
H11	–Bc11	–Bc6	117.7	H21	–Cc21	–Bc27	116.2
H11	–Bc11	–Bc7	115.5	H22	–Cc22	–Cc21	117.6
H11	–Bc11	–Bc8	122.2	H22	–Cc22	–Bc23	121.8
H11	–Bc11	–Bc9	127.2	H22	–Cc22	–Bc27	112.7
H11	–Bc11	–Bc10	124.6	H22	–Cc22	–Bc28	116.9
H16A	–Cp16	–Cp11	115.0	H23	–Bc23	–Cc22	127.6
H16B	–Cp16	–Cp11	108.7	H23	–Bc23	–Bc24	118.1
H16C	–Cp16	–Cp11	110.4	H23	–Bc23	–Bc28	121.5
H16B	–Cp16	–H16A	108.5	H23	–Bc23	–Bc29	117.4
H16C	–Cp16	–H16A	110.2	H24	–Bc24	–Bc23	120.8
H16C	–Cp16	–H16B	103.4	H24	–Bc24	–Bc25	122.7

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Table S3. (Cont.)

	Angle(°)		Angle(°)
H24 –Bc24 –Bc29	121.6	Li1 –O1 –C4	127.3(21)
H24 –Bc24 –Bc30	121.4	C4 –C1 –C2	99.1(38)
H25 –Bc25 –Cc21	123.4	C3 –C2 –C1	119.5(47)
H25 –Bc25 –Bc24	123.8	C2 –C3 –O1	102.2(31)
H25 –Bc25 –Bc26	118.2	C1 –C4 –O1	105.5(24)
H25 –Bc25 –Bc30	118.4	C8 –O2 –C5	92.8(38)
H26 –Bc26 –Cc21	123.9	C6 –C5 –O2	102.8(26)
H26 –Bc26 –Bc25	119.6	C8 –C5 –O2	31.2(20)
H26 –Bc26 –Bc27	123.6	C8 –C5 –C6	71.7(25)
H26 –Bc26 –Bc30	121.3	C7 –C6 –C5	104.6(29)
H26 –Bc26 –Bc31	125.6	C8 –C7 –C6	86.6(31)
H27 –Bc27 –Cc21	121.9	C5 –C8 –O2	56.0(31)
H27 –Bc27 –Cc22	125.6	C7 –C8 –O2	129.3(50)
H27 –Bc27 –Bc26	120.3	C7 –C8 –C5	83.2(29)
H27 –Bc27 –Bc28	125.8	Cs3 –Cs2 –Cs1	119.6
H27 –Bc27 –Bc31	126.2	Cs7 –Cs2 –Cs1	118.7
H28 –Bc28 –Cc22	125.8	Cs7 –Cs2 –Cs3	121.6
H28 –Bc28 –Bc23	129.6	Cs4 –Cs3 –Cs2	118.9
H28 –Bc28 –Bc27	114.6	Cs5 –Cs4 –Cs3	120.4
H28 –Bc28 –Bc29	124.8	Cs6 –Cs5 –Cs4	120.3
H28 –Bc28 –Bc31	118.4	Cs7 –Cs6 –Cs5	120.6
H29 –Bc29 –Bc23	124.5	Cs6 –Cs7 –Cs2	118.3
H29 –Bc29 –Bc24	118.2	Cs13 –Cs12 –Cs11	119.8
H29 –Bc29 –Bc28	127.0	Cs17 –Cs12 –Cs11	120.4
H29 –Bc29 –Bc30	118.2	Cs17 –Cs12 –Cs13	119.8
H29 –Bc29 –Bc31	124.6	Cs14 –Cs13 –Cs12	118.5
H30 –Bc30 –Bc24	126.4	Cs15 –Cs14 –Cs13	121.3
H30 –Bc30 –Bc25	121.6	Cs16 –Cs15 –Cs14	120.0
H30 –Bc30 –Bc26	117.9	Cs17 –Cs16 –Cs15	120.3
H30 –Bc30 –Bc29	126.9	Cs16 –Cs17 –Cs12	120.0
H30 –Bc30 –Bc31	121.8	Cs23 –Cs22 –Cs21	119.6
H31 –Bc31 –Bc26	120.3	Cs27 –Cs22 –Cs21	120.3
H31 –Bc31 –Bc27	121.5	Cs27 –Cs22 –Cs23	120.2
H31 –Bc31 –Bc28	122.9	Cs24 –Cs23 –Cs22	120.3
H31 –Bc31 –Bc29	121.5	Cs25 –Cs24 –Cs23	118.2
H31 –Bc31 –Bc30	120.9	Cs26 –Cs25 –Cs24	121.5
C4 –O1 –C3	112.3(20)	Cs27 –Cs26 –Cs25	119.9
Li1 –O1 –C3	120.3(23)	Cs26 –Cs27 –Cs22	119.9