Electronic Supplementary Information (ESI)

The Reaction of bis(1,2,4-tri-t-butylcyclopentadienyl)ceriumbenzyl, Cp'_2CeCH_2Ph with Methylhalides: a Metathesis Reaction that does not proceed by a Metathesis Transition State.

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Index to supporting information

1. $Cp'_2CeCH_2C_6H_5$

A fragment of a red block-like crystal of bis(tri-t-butylcyclopentadienyl)cerium benzyl having approximate dimensions of 0.30 x 0.27 x 0.10 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker SMART 1000 CCD [10] area detector with graphite monochromated MoKα radiation. Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 8192 centered reflections with $I > 10\sigma(I)$ in the range $1.15 < \theta < 25.99^o$ corresponded to a primitive Triclinic cell with dimensions:

a = 13.228(1) Å	α = 96.377(1) ^{o}
b = 16.080(1) Å	β = 105.388(1) ^{o}
c = 18.499(1) Å	γ = 96.173(1) ^{o}
V = 3731.57(14) Å^3	

For Z = 4 and F.W. = 698.05, the calculated density is 1.243 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be $P\bar{1}$ (#2). The data were collected at a temperature of -94 ± 1^{o}C. using 10 second scans 0.3^o wide in ω. Data were integrated by the program SAINT[11] to a maximum θ value of 25.00^o. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 0.8856, Tmin = 0.7065). Of the 17828 reflections that were collected, 12450 were unique (R_{int} = 0.0229); equivalent reflections were merged. No decay correction was applied.

The structure was solved by direct methods[1] and expanded using Fourier techniques[2,15]. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[3] was based on 12450 reflections (all data) and 793 variable parameters and

converged (largest parameter shift was 0.002 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0361 \text{ for } 10075 \text{ data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.0707$$

The standard deviation of an observation of unit weight[4] was 1.085. The weighting scheme was based on counting statistics and included a factor (p = 0.030) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.669 and -0.954 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. Calculations were performed using were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation and the SHELXTL[16] crystallographic software package of Bruker Analytical X-ray Systems Inc.
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1.1 Atomic coordinates and B_{iso}/B_{eq} for $Cp'_2CeCH_2C_6H_5$

atom	x	y	z	U_{eq}	Occupancy
C1	0.4757(3)	0.2145(3)	0.4472(2)	0.024(1)	1
C2	0.5752(3)	0.2512(2)	0.5007(2)	0.026(1)	1
C3	0.6456(3)	0.1900(2)	0.4991(2)	0.025(1)	1
C4	0.5934(3)	0.1167(2)	0.4490(2)	0.024(1)	1
C5	0.4901(3)	0.1335(2)	0.4161(2)	0.024(1)	1
C6	0.3633(3)	0.2405(3)	0.4311(2)	0.030(1)	1
C7	0.3258(3)	0.2415(3)	0.5034(3)	0.037(1)	1
C8	0.3558(3)	0.3264(3)	0.4016(3)	0.034(1)	1
C9	0.2826(3)	0.1757(3)	0.3707(3)	0.037(1)	1
C10	0.6075(3)	0.3234(3)	0.5694(2)	0.033(1)	1
C11	0.5506(4)	0.4021(3)	0.5616(3)	0.043(1)	1
C12	0.5875(4)	0.2839(3)	0.6377(2)	0.044(1)	1
C13	0.7260(4)	0.3571(3)	0.5908(3)	0.043(1)	1
C14	0.6410(3)	0.0364(2)	0.4337(2)	0.025(1)	1
C15	0.5536(4)	-0.0397(3)	0.4023(3)	0.036(1)	1
C16	0.7031(3)	0.0487(3)	0.3752(2)	0.032(1)	1
C17	0.7181(4)	0.0193(3)	0.5069(2)	0.040(1)	1
C18	0.8577(3)	0.2841(3)	0.3801(2)	0.029(1)	1
C19	0.8193(3)	0.2641(2)	0.2986(2)	0.026(1)	1

C20	0.7467(3)	0.3212(2)	0.2739(2)	0.027(1)	1
C21	0.7406(3)	0.3781(3)	0.3355(2)	0.029(1)	1
C22	0.8053(3)	0.3534(3)	0.4000(3)	0.033(1)	1
C23	0.9552(3)	0.2657(3)	0.4404(3)	0.041(1)	1
C24	0.9383(4)	0.2789(5)	0.5199(3)	0.072(2)	1
C25	1.0486(4)	0.3323(3)	0.4413(3)	0.058(2)	1
C26	0.9861(4)	0.1763(3)	0.4312(3)	0.049(1)	1
C27	0.8570(3)	0.2058(3)	0.2416(2)	0.032(1)	1
C28	0.8305(4)	0.1111(3)	0.2449(3)	0.042(1)	1
C29	0.9765(3)	0.2301(3)	0.2517(3)	0.044(1)	1
C30	0.8025(4)	0.2185(3)	0.1599(2)	0.042(1)	1
C31	0.6762(3)	0.4520(3)	0.3350(3)	0.037(1)	1
C32	0.7452(4)	0.5301(3)	0.3879(4)	0.063(2)	1
C33	0.5830(4)	0.4261(3)	0.3657(3)	0.044(1)	1
C34	0.6352(4)	0.4736(3)	0.2556(3)	0.058(2)	1
C35	0.4677(3)	0.2367(3)	0.2398(2)	0.037(1)	1
C36	0.4879(3)	0.1651(3)	0.1950(2)	0.034(1)	1
C37	0.5198(4)	0.1709(3)	0.1280(3)	0.046(1)	1
C38	0.5427(4)	0.1010(4)	0.0880(3)	0.058(2)	1
C39	0.5389(4)	0.0227(4)	0.1126(3)	0.057(2)	1
C40	0.5102(4)	0.0155(3)	0.1777(3)	0.053(1)	1
C41	0.4852(4)	0.0843(3)	0.2179(3)	0.042(1)	1
C42	0.2858(3)	0.3349(2)	-0.1318(2)	0.025(1)	1
C43	0.2260(3)	0.2828(3)	-0.2012(2)	0.028(1)	1
C44	0.1355(3)	0.3217(2)	-0.2315(2)	0.028(1)	1
C45	0.1386(3)	0.3987(3)	-0.1858(2)	0.026(1)	1
C46	0.2303(3)	0.4062(2)	-0.1242(2)	0.028(1)	1
C47	0.2514(3)	0.2055(3)	-0.2472(2)	0.033(1)	1
C48	0.2541(4)	0.1266(3)	-0.2075(3)	0.040(1)	1
C49	0.3554(4)	0.2287(3)	-0.2675(3)	0.043(1)	1
C50	0.1669(4)	0.1814(3)	-0.3246(2)	0.045(1)	1
C51	0.3988(3)	0.3395(3)	-0.0775(2)	0.031(1)	1
C52	0.4755(3)	0.3950(3)	-0.1090(3)	0.041(1)	1
C53	0.4429(3)	0.2552(3)	-0.0672(2)	0.035(1)	1
C54	0.4057(3)	0.3826(3)	0.0020(2)	0.040(1)	1
C55	0.0547(3)	0.4578(3)	-0.2002(2)	0.031(1)	1
C56	0.0257(4)	0.4736(3)	-0.2832(3)	0.048(1)	1
C57	0.0965(4)	0.5438(3)	-0.1496(3)	0.043(1)	1
C58	-0.0463(3)	0.4189(3)	-0.1837(2)	0.032(1)	1
C59	-0.0809(3)	0.1357(2)	-0.1544(2)	0.026(1)	1
C60	-0.1106(3)	0.1868(2)	-0.0965(2)	0.026(1)	1
C61	-0.0319(3)	0.1859(3)	-0.0268(2)	0.026(1)	1
C62	0.0453(3)	0.1351(3)	-0.0385(2)	0.029(1)	1
C63	0.0153(3)	0.1068(3)	-0.1171(2)	0.030(1)	1
C64	-0.1369(3)	0.1030(3)	-0.2387(2)	0.032(1)	1
C65	-0.0769(4)	0.0388(3)	-0.2714(3)	0.042(1)	1

C66	-0.1453(4)	0.1738(3)	-0.2882(2)	0.039(1)	1
C67	-0.2481(3)	0.0538(3)	-0.2489(3)	0.043(1)	1
C68	-0.2141(3)	0.2235(3)	-0.0941(2)	0.029(1)	1
C69	-0.2749(3)	0.2554(3)	-0.1659(2)	0.038(1)	1
C70	-0.2866(3)	0.1529(3)	-0.0744(3)	0.039(1)	1
C71	-0.1923(3)	0.2993(3)	-0.0309(2)	0.037(1)	1
C72	0.1454(3)	0.1217(3)	0.0198(2)	0.032(1)	1
C73	0.1247(4)	0.1155(3)	0.0970(3)	0.049(1)	1
C74	0.2308(3)	0.1976(3)	0.0291(2)	0.037(1)	1
C75	0.1862(4)	0.0412(3)	-0.0060(3)	0.055(1)	1
C76	0.0945(4)	0.3951(3)	0.0095(2)	0.035(1)	1
C77	0.1633(3)	0.4121(3)	0.0875(2)	0.028(1)	1
C78	0.2516(3)	0.4753(3)	0.1112(3)	0.036(1)	1
C79	0.3166(4)	0.4894(3)	0.1855(3)	0.045(1)	1
C80	0.2954(4)	0.4410(3)	0.2381(3)	0.047(1)	1
C81	0.2086(4)	0.3785(3)	0.2166(3)	0.041(1)	1
C82	0.1452(3)	0.3646(3)	0.1432(2)	0.033(1)	1
Ce1	0.6290(1)	0.2301(1)	0.3531(1)	0.023(1)	1
Ce2	0.0886(1)	0.2793(1)	-0.1003(1)	0.023(1)	1
H3	0.7178	0.1978	0.5279	0.030	1
H5	0.4374	0.0956	0.3782	0.028	1
H7A	0.2512	0.2498	0.4914	0.056	1
H7B	0.3687	0.2877	0.5419	0.056	1
H7C	0.3338	0.1875	0.5228	0.056	1
H8A	0.3650	0.3213	0.3505	0.051	1
H8B	0.4115	0.3693	0.4354	0.051	1
H8C	0.2863	0.3431	0.4000	0.051	1
H9A	0.2791	0.1208	0.3888	0.056	1
H9B	0.3043	0.1705	0.3239	0.056	1
H9C	0.2128	0.1945	0.3608	0.056	1
H11A	0.5775	0.4422	0.6085	0.064	1
H11B	0.4743	0.3852	0.5519	0.064	1
H11C	0.5640	0.4289	0.5193	0.064	1
H12A	0.6096	0.3269	0.6829	0.066	1
H12B	0.6284	0.2369	0.6465	0.066	1
H12C	0.5119	0.2631	0.6270	0.066	1
H13A	0.7426	0.3817	0.5484	0.064	1
H13B	0.7672	0.3107	0.6022	0.064	1
H13C	0.7441	0.4006	0.6355	0.064	1
H15A	0.5136	-0.0479	0.4392	0.054	1
H15B	0.5857	-0.0905	0.3927	0.054	1
H15C	0.5058	-0.0294	0.3548	0.054	1
H16A	0.6539	0.0545	0.3266	0.048	1
H16B	0.7393	-0.0005	0.3685	0.048	1
H16C	0.7555	0.0997	0.3932	0.048	1
H17A	0.7772	0.0658	0.5244	0.059	1

H17B	0.7454	-0.0338	0.4970	0.059	1
H17C	0.6810	0.0152	0.5460	0.059	1
H20	0.7076	0.3209	0.2228	0.032	1
H22	0.8135	0.3790	0.4505	0.039	1
H24A	0.9267	0.3374	0.5319	0.107	1
H24B	1.0011	0.2676	0.5574	0.107	1
H24C	0.8763	0.2402	0.5209	0.107	1
H25A	1.0670	0.3224	0.3934	0.088	1
H25B	1.1099	0.3280	0.4835	0.088	1
H25C	1.0283	0.3890	0.4475	0.088	1
H26A	0.9286	0.1348	0.4353	0.073	1
H26B	1.0509	0.1733	0.4710	0.073	1
H26C	0.9984	0.1638	0.3814	0.073	1
H28A	0.7534	0.0954	0.2309	0.063	1
H28B	0.8615	0.0996	0.2965	0.063	1
H28C	0.8596	0.0781	0.2095	0.063	1
H29A	1.0168	0.2189	0.3015	0.066	1
H29B	0.9914	0.2903	0.2482	0.066	1
H29C	0.9972	0.1965	0.2119	0.066	1
H30A	0.8251	0.1800	0.1243	0.063	1
H30B	0.8222	0.2771	0.1531	0.063	1
H30C	0.7255	0.2066	0.1502	0.063	1
H32A	0.7682	0.5167	0.4397	0.094	1
H32B	0.7038	0.5772	0.3871	0.094	1
H32C	0.8074	0.5460	0.3705	0.094	1
H33A	0.5366	0.3778	0.3317	0.067	1
H33B	0.5430	0.4736	0.3689	0.067	1
H33C	0.6095	0.4102	0.4163	0.067	1
H34A	0.6951	0.4899	0.2359	0.087	1
H34B	0.5941	0.5207	0.2571	0.087	1
H34C	0.5898	0.4242	0.2225	0.087	1
H35A	0.3993	0.2270	0.2520	0.044	1
H35B	0.4734	0.2895	0.2174	0.044	1
H37	0.5255	0.2240	0.1104	0.056	1
H38	0.5614	0.1068	0.0424	0.069	1
H39	0.5558	-0.0247	0.0850	0.068	1
H40	0.5075	-0.0376	0.1957	0.063	1
H41	0.4653	0.0768	0.2627	0.051	1
H44	0.0806	0.2990	-0.2763	0.033	1
H46	0.2522	0.4517	-0.0836	0.034	1
H48A	0.2801	0.0824	-0.2356	0.059	1
H48B	0.1825	0.1060	-0.2055	0.059	1
H48C	0.3013	0.1410	-0.1558	0.059	1
H49A	0.4146	0.2403	-0.2211	0.065	1
H49B	0.3512	0.2792	-0.2928	0.065	1
H49C	0.3667	0.1816	-0.3015	0.065	1

H50A	0.1672	0.2286	-0.3538	0.068	1
H50B	0.0969	0.1688	-0.3165	0.068	1
H50C	0.1829	0.1314	-0.3525	0.068	1
H52A	0.4537	0.4512	-0.1117	0.062	1
H52B	0.4736	0.3686	-0.1598	0.062	1
H52C	0.5476	0.4004	-0.0754	0.062	1
H53A	0.5137	0.2663	-0.0312	0.052	1
H53B	0.4471	0.2278	-0.1161	0.052	1
H53C	0.3958	0.2181	-0.0477	0.052	1
H54A	0.4773	0.3836	0.0353	0.059	1
H54B	0.3542	0.3511	0.0220	0.059	1
H54C	0.3903	0.4406	-0.0005	0.059	1
H56A	0.0882	0.5019	-0.2941	0.072	1
H56B	-0.0306	0.5094	-0.2918	0.072	1
H56C	0.0008	0.4194	-0.3167	0.072	1
H57A	0.1115	0.5358	-0.0962	0.064	1
H57B	0.0430	0.5817	-0.1609	0.064	1
H57C	0.1616	0.5685	-0.1595	0.064	1
H58A	-0.0726	0.3637	-0.2152	0.048	1
H58B	-0.1004	0.4563	-0.1951	0.048	1
H58C	-0.0305	0.4117	-0.1301	0.048	1
H61	-0.0313	0.2153	0.0208	0.032	1
H63	0.0541	0.0729	-0.1420	0.036	1
H65A	-0.1141	0.0192	-0.3249	0.063	1
H65B	-0.0732	-0.0095	-0.2433	0.063	1
H65C	-0.0050	0.0657	-0.2669	0.063	1
H66A	-0.0741	0.1993	-0.2870	0.059	1
H66B	-0.1821	0.2170	-0.2687	0.059	1
H66C	-0.1850	0.1503	-0.3404	0.059	1
H67A	-0.2925	0.0918	-0.2311	0.064	1
H67B	-0.2416	0.0067	-0.2194	0.064	1
H67C	-0.2808	0.0318	-0.3026	0.064	1
H69A	-0.2993	0.2081	-0.2076	0.057	1
H69B	-0.2282	0.2989	-0.1793	0.057	1
H69C	-0.3362	0.2794	-0.1567	0.057	1
H70A	-0.3534	0.1729	-0.0726	0.058	1
H70B	-0.2513	0.1379	-0.0249	0.058	1
H70C	-0.3011	0.1030	-0.1131	0.058	1
H71A	-0.1492	0.3464	-0.0428	0.055	1
H71B	-0.1541	0.2831	0.0174	0.055	1
H71C	-0.2596	0.3166	-0.0268	0.055	1
H73A	0.0979	0.1666	0.1136	0.074	1
H73B	0.1909	0.1099	0.1343	0.074	1
H73C	0.0722	0.0659	0.0925	0.074	1
H74A	0.2456	0.2020	-0.0196	0.055	1
H74B	0.2956	0.1899	0.0667	0.055	1

H74C	0.2057	0.2494	0.0461	0.055	1
H75A	0.1315	-0.0076	-0.0132	0.082	1
H75B	0.2501	0.0335	0.0325	0.082	1
H75C	0.2032	0.0462	-0.0540	0.082	1
H76A	0.1037	0.4489	-0.0109	0.042	1
H76B	0.0216	0.3887	0.0148	0.042	1
H78	0.2675	0.5094	0.0757	0.044	1
H79	0.3759	0.5327	0.2000	0.053	1
H80	0.3401	0.4505	0.2887	0.056	1
H81	0.1927	0.3451	0.2525	0.049	1
H82	0.0864	0.3209	0.1295	0.040	1

1.2 Anisotropic Displacement Parameters for $Cp'_2CeCH_2C_6H_5$

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.026(2)	0.029(2)	0.021(2)	0.007(2)	0.009(2)	0.006(2)
C2	0.032(2)	0.026(2)	0.027(2)	0.008(2)	0.014(2)	0.011(2)
C3	0.027(2)	0.027(2)	0.023(2)	0.005(2)	0.008(2)	0.012(2)
C4	0.033(2)	0.023(2)	0.023(2)	0.010(2)	0.014(2)	0.011(2)
C5	0.025(2)	0.027(2)	0.020(2)	0.007(2)	0.007(2)	0.002(2)
C6	0.027(2)	0.032(2)	0.034(2)	0.007(2)	0.014(2)	0.009(2)
C7	0.032(2)	0.043(3)	0.048(3)	0.016(2)	0.021(2)	0.019(2)
C8	0.031(2)	0.034(2)	0.045(3)	0.016(2)	0.015(2)	0.016(2)
C9	0.025(2)	0.039(3)	0.048(3)	0.008(2)	0.010(2)	0.004(2)
C10	0.040(3)	0.034(2)	0.026(2)	-0.002(2)	0.009(2)	0.014(2)
C11	0.048(3)	0.032(3)	0.044(3)	-0.010(2)	0.006(2)	0.015(2)
C12	0.054(3)	0.053(3)	0.029(2)	0.001(2)	0.015(2)	0.019(3)
C13	0.043(3)	0.042(3)	0.036(3)	-0.010(2)	0.005(2)	0.009(2)
C14	0.035(2)	0.021(2)	0.023(2)	0.003(2)	0.012(2)	0.010(2)
C15	0.047(3)	0.025(2)	0.042(3)	0.004(2)	0.021(2)	0.008(2)
C16	0.037(3)	0.029(2)	0.037(2)	0.005(2)	0.019(2)	0.013(2)
C17	0.050(3)	0.038(3)	0.034(3)	0.011(2)	0.009(2)	0.025(2)
C18	0.021(2)	0.030(2)	0.034(2)	0.000(2)	0.008(2)	0.003(2)
C19	0.022(2)	0.021(2)	0.038(2)	0.003(2)	0.014(2)	0.002(2)
C20	0.029(2)	0.027(2)	0.028(2)	0.007(2)	0.013(2)	0.001(2)
C21	0.022(2)	0.024(2)	0.042(3)	0.005(2)	0.013(2)	0.000(2)
C22	0.026(2)	0.033(2)	0.038(3)	-0.004(2)	0.012(2)	0.002(2)
C23	0.025(2)	0.053(3)	0.040(3)	-0.002(2)	0.004(2)	0.010(2)
C24	0.040(3)	0.136(6)	0.035(3)	0.005(3)	-0.001(2)	0.035(4)
C25	0.024(3)	0.055(3)	0.084(4)	-0.007(3)	0.001(3)	0.007(2)
C26	0.033(3)	0.058(3)	0.055(3)	0.018(3)	0.006(2)	0.013(2)
C27	0.037(3)	0.028(2)	0.039(3)	0.006(2)	0.022(2)	0.005(2)
C28	0.057(3)	0.030(2)	0.048(3)	0.006(2)	0.030(2)	0.010(2)
C29	0.039(3)	0.042(3)	0.062(3)	0.009(2)	0.030(2)	0.009(2)
C30	0.058(3)	0.038(3)	0.039(3)	0.005(2)	0.028(2)	0.007(2)

C31	0.034(3)	0.025(2)	0.060(3)	0.007(2)	0.023(2)	0.010(2)
C32	0.056(3)	0.029(3)	0.106(5)	-0.011(3)	0.036(3)	0.006(3)
C33	0.036(3)	0.041(3)	0.065(3)	0.006(3)	0.024(2)	0.016(2)
C34	0.067(4)	0.048(3)	0.079(4)	0.030(3)	0.037(3)	0.030(3)
C35	0.029(2)	0.042(3)	0.036(3)	0.007(2)	0.006(2)	0.001(2)
C36	0.027(2)	0.047(3)	0.025(2)	0.006(2)	0.000(2)	0.002(2)
C37	0.044(3)	0.060(3)	0.030(3)	0.010(2)	0.005(2)	-0.001(3)
C38	0.044(3)	0.089(5)	0.034(3)	-0.007(3)	0.013(2)	-0.006(3)
C39	0.052(3)	0.062(4)	0.044(3)	-0.018(3)	0.007(3)	0.002(3)
C40	0.060(3)	0.047(3)	0.042(3)	-0.002(3)	0.004(3)	0.003(3)
C41	0.041(3)	0.050(3)	0.033(3)	0.003(2)	0.009(2)	0.000(2)
C42	0.025(2)	0.024(2)	0.028(2)	0.006(2)	0.011(2)	0.005(2)
C43	0.032(2)	0.027(2)	0.032(2)	0.008(2)	0.016(2)	0.006(2)
C44	0.029(2)	0.027(2)	0.028(2)	0.004(2)	0.011(2)	0.005(2)
C45	0.025(2)	0.027(2)	0.030(2)	0.010(2)	0.012(2)	0.004(2)
C46	0.034(2)	0.021(2)	0.033(2)	0.004(2)	0.015(2)	0.004(2)
C47	0.038(3)	0.030(2)	0.036(2)	0.004(2)	0.018(2)	0.012(2)
C48	0.046(3)	0.027(2)	0.049(3)	0.000(2)	0.017(2)	0.015(2)
C49	0.049(3)	0.044(3)	0.045(3)	0.001(2)	0.027(2)	0.012(2)
C50	0.057(3)	0.042(3)	0.036(3)	-0.005(2)	0.012(2)	0.019(3)
C51	0.026(2)	0.030(2)	0.038(2)	0.007(2)	0.010(2)	0.003(2)
C52	0.028(2)	0.040(3)	0.056(3)	0.012(2)	0.012(2)	-0.003(2)
C53	0.027(2)	0.040(3)	0.040(3)	0.014(2)	0.008(2)	0.012(2)
C54	0.033(3)	0.040(3)	0.040(3)	0.001(2)	0.002(2)	0.003(2)
C55	0.032(2)	0.030(2)	0.038(2)	0.012(2)	0.016(2)	0.014(2)
C56	0.050(3)	0.061(3)	0.048(3)	0.030(3)	0.021(2)	0.029(3)
C57	0.042(3)	0.023(2)	0.067(3)	0.007(2)	0.019(2)	0.008(2)
C58	0.029(2)	0.031(2)	0.039(3)	0.009(2)	0.012(2)	0.009(2)
C59	0.024(2)	0.023(2)	0.028(2)	0.008(2)	0.004(2)	0.000(2)
C60	0.023(2)	0.025(2)	0.029(2)	0.010(2)	0.005(2)	0.003(2)
C61	0.025(2)	0.028(2)	0.026(2)	0.005(2)	0.005(2)	0.002(2)
C62	0.024(2)	0.025(2)	0.036(2)	0.011(2)	0.006(2)	0.001(2)
C63	0.031(2)	0.023(2)	0.039(3)	0.007(2)	0.012(2)	0.003(2)
C64	0.026(2)	0.032(2)	0.033(2)	0.001(2)	0.005(2)	0.002(2)
C65	0.041(3)	0.041(3)	0.036(3)	-0.004(2)	0.004(2)	0.006(2)
C66	0.046(3)	0.041(3)	0.029(2)	0.006(2)	0.009(2)	0.001(2)
C67	0.038(3)	0.041(3)	0.041(3)	0.003(2)	0.002(2)	-0.004(2)
C68	0.022(2)	0.035(2)	0.032(2)	0.010(2)	0.008(2)	0.002(2)
C69	0.032(3)	0.045(3)	0.039(3)	0.010(2)	0.009(2)	0.012(2)
C70	0.029(2)	0.040(3)	0.050(3)	0.013(2)	0.013(2)	0.005(2)
C71	0.029(2)	0.041(3)	0.042(3)	0.007(2)	0.012(2)	0.013(2)
C72	0.031(2)	0.031(2)	0.035(2)	0.016(2)	0.005(2)	0.005(2)
C73	0.044(3)	0.062(3)	0.044(3)	0.033(3)	0.005(2)	0.009(3)
C74	0.028(2)	0.042(3)	0.040(3)	0.016(2)	0.004(2)	0.007(2)
C75	0.052(3)	0.041(3)	0.063(3)	0.011(3)	-0.005(3)	0.022(3)
C76	0.043(3)	0.033(2)	0.032(2)	0.007(2)	0.015(2)	0.005(2)

C77	0.028(2)	0.025(2)	0.033(2)	0.002(2)	0.012(2)	0.008(2)
C78	0.038(3)	0.030(2)	0.044(3)	0.003(2)	0.018(2)	0.000(2)
C79	0.028(3)	0.042(3)	0.057(3)	-0.001(3)	0.007(2)	-0.002(2)
C80	0.044(3)	0.047(3)	0.039(3)	0.001(2)	-0.002(2)	0.005(2)
C81	0.051(3)	0.039(3)	0.033(3)	0.011(2)	0.009(2)	0.005(2)
C82	0.031(2)	0.032(2)	0.035(2)	0.004(2)	0.009(2)	0.001(2)
Ce1	0.023(1)	0.025(1)	0.023(1)	0.006(1)	0.008(1)	0.005(1)
Ce2	0.025(1)	0.021(1)	0.023(1)	0.005(1)	0.008(1)	0.003(1)

The general temperature factor expression:

$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$

1.3 Bond Lengths(Å) for $Cp'_2CeCH_2C_6H_5$

atom	atom	distance	atom	atom	distance
C1	C5	1.418(5)	C1	C2	1.439(5)
C1	C6	1.549(5)	C1	Ce1	3.010(4)
C2	C3	1.429(5)	C2	C10	1.556(5)
C2	Ce1	2.992(4)	C3	C4	1.402(5)
C3	Ce1	2.803(4)	C3	H3	0.9500
C4	C5	1.407(5)	C4	C14	1.528(5)
C4	Ce1	2.769(4)	C5	Ce1	2.840(4)
C5	H5	0.9500	C6	C9	1.530(6)
C6	C7	1.544(5)	C6	C8	1.544(6)
C7	H7A	0.9800	C7	H7B	0.9800
C7	H7C	0.9800	C8	H8A	0.9800
C8	H8B	0.9800	C8	H8C	0.9800
C9	H9A	0.9800	C9	H9B	0.9800
C9	H9C	0.9800	C10	C13	1.533(6)
C10	C11	1.542(6)	C10	C12	1.546(6)
C11	H11A	0.9800	C11	H11B	0.9800
C11	H11C	0.9800	C12	H12A	0.9800
C12	H12B	0.9800	C12	H12C	0.9800
C13	H13A	0.9800	C13	H13B	0.9800
C13	H13C	0.9800	C14	C15	1.534(6)
C14	C17	1.536(5)	C14	C16	1.540(5)
C15	H15A	0.9800	C15	H15B	0.9800
C15	H15C	0.9800	C16	H16A	0.9800
C16	H16B	0.9800	C16	H16C	0.9800
C17	H17A	0.9800	C17	H17B	0.9800
C17	H17C	0.9800	C18	C22	1.440(5)
C18	C19	1.444(6)	C18	C23	1.545(6)
C18	Ce1	2.949(4)	C19	C20	1.422(5)
C19	C27	1.550(5)	C19	Ce1	2.970(4)

C20	C21	1.404(5)	C20	Ce1	2.813(4)
C20	H20	0.9500	C21	C22	1.397(6)
C21	C31	1.534(6)	C21	Ce1	2.761(4)
C22	Ce1	2.770(4)	C22	H22	0.9500
C23	C24	1.540(6)	C23	C26	1.540(6)
C23	C25	1.542(7)	C24	H24A	0.9800
C24	H24B	0.9800	C24	H24C	0.9800
C25	H25A	0.9800	C25	H25B	0.9800
C25	H25C	0.9800	C26	H26A	0.9800
C26	H26B	0.9800	C26	H26C	0.9800
C27	C28	1.537(6)	C27	C30	1.539(6)
C27	C29	1.542(6)	C28	H28A	0.9800
C28	H28B	0.9800	C28	H28C	0.9800
C29	H29A	0.9800	C29	H29B	0.9800
C29	H29C	0.9800	C30	H30A	0.9800
C30	H30B	0.9800	C30	H30C	0.9800
C31	C34	1.519(7)	C31	C33	1.526(6)
C31	C32	1.540(6)	C32	H32A	0.9800
C32	H32B	0.9800	C32	H32C	0.9800
C33	H33A	0.9800	C33	H33B	0.9800
C33	H33C	0.9800	C34	H34A	0.9800
C34	H34B	0.9800	C34	H34C	0.9800
C35	C36	1.434(6)	C35	Ce1	2.584(4)
C35	H35A	0.9900	C35	H35B	0.9900
C36	C41	1.409(6)	C36	C37	1.420(6)
C36	Ce1	3.023(4)	C37	C38	1.382(7)
C37	H37	0.9500	C38	C39	1.386(8)
C38	H38	0.9500	C39	C40	1.369(7)
C39	H39	0.9500	C40	C41	1.383(7)
C40	H40	0.9500	C41	H41	0.9500
C42	C43	1.434(6)	C42	C46	1.439(5)
C42	C51	1.553(6)	C42	Ce2	2.893(4)
C43	C44	1.422(5)	C43	C47	1.546(5)
C43	Ce2	2.932(4)	C44	C45	1.410(5)
C44	Ce2	2.795(4)	C44	H44	0.9500
C45	C46	1.410(6)	C45	C55	1.526(5)
C45	Ce2	2.752(4)	C46	Ce2	2.773(4)
C46	H46	0.9500	C47	C48	1.535(6)
C47	C49	1.539(6)	C47	C50	1.543(6)
C48	H48A	0.9800	C48	H48B	0.9800
C48	H48C	0.9800	C49	H49A	0.9800
C49	H49B	0.9800	C49	H49C	0.9800
C50	H50A	0.9800	C50	H50B	0.9800
C50	H50C	0.9800	C51	C54	1.529(6)
C51	C53	1.543(6)	C51	C52	1.549(6)
C52	H52A	0.9800	C52	H52B	0.9800

C52	H52C	0.9800	C53	H53A	0.9800
C53	H53B	0.9800	C53	H53C	0.9800
C54	H54A	0.9800	C54	H54B	0.9800
C54	H54C	0.9800	C55	C58	1.533(5)
C55	C57	1.538(6)	C55	C56	1.539(6)
C56	H56A	0.9800	C56	H56B	0.9800
C56	H56C	0.9800	C57	H57A	0.9800
C57	H57B	0.9800	C57	H57C	0.9800
C58	H58A	0.9800	C58	H58B	0.9800
C58	H58C	0.9800	C59	C63	1.430(5)
C59	C60	1.440(5)	C59	C64	1.542(5)
C59	Ce2	2.923(4)	C60	C61	1.428(5)
C60	C68	1.558(5)	C60	Ce2	2.904(4)
C61	C62	1.421(5)	C61	Ce2	2.781(4)
C61	H61	0.9500	C62	C63	1.408(6)
C62	C72	1.523(5)	C62	Ce2	2.769(4)
C63	Ce2	2.793(4)	C63	H63	0.9500
C64	C65	1.534(6)	C64	C66	1.534(6)
C64	C67	1.548(6)	C65	H65A	0.9800
C65	H65B	0.9800	C65	H65C	0.9800
C66	H66A	0.9800	C66	H66B	0.9800
C66	H66C	0.9800	C67	H67A	0.9800
C67	H67B	0.9800	C67	H67C	0.9800
C68	C69	1.531(6)	C68	C71	1.538(6)
C68	C70	1.545(6)	C69	H69A	0.9800
C69	H69B	0.9800	C69	H69C	0.9800
C70	H70A	0.9800	C70	H70B	0.9800
C70	H70C	0.9800	C71	H71A	0.9800
C71	H71B	0.9800	C71	H71C	0.9800
C72	C74	1.532(6)	C72	C75	1.532(6)
C72	C73	1.536(6)	C73	H73A	0.9800
C73	H73B	0.9800	C73	H73C	0.9800
C74	H74A	0.9800	C74	H74B	0.9800
C74	H74C	0.9800	C75	H75A	0.9800
C75	H75B	0.9800	C75	H75C	0.9800
C76	C77	1.465(6)	C76	Ce2	2.577(4)
C76	H76A	0.9900	C76	H76B	0.9900
C77	C78	1.401(6)	C77	C82	1.404(6)
C78	C79	1.394(6)	C78	H78	0.9500
C79	C80	1.377(7)	C79	H79	0.9500
C80	C81	1.382(6)	C80	H80	0.9500
C81	C82	1.371(6)	C81	H81	0.9500
C82	H82	0.9500			

1.4 Bond Angles(°) for $Cp'_2CeCH_2C_6H_5$

atom	atom	atom	angle	atom	atom	atom	angle
C5	C1	C2	106.6(3)	C5	C1	C6	120.1(3)
C2	C1	C6	132.3(3)	C5	C1	Ce1	69.4(2)
C2	C1	Ce1	75.4(2)	C6	C1	Ce1	128.1(2)
C3	C2	C1	106.1(3)	C3	C2	C10	117.3(3)
C1	C2	C10	133.7(3)	C3	C2	Ce1	68.5(2)
C1	C2	Ce1	76.8(2)	C10	C2	Ce1	132.8(3)
C4	C3	C2	110.6(4)	C4	C3	Ce1	74.1(2)
C2	C3	Ce1	83.2(2)	C4	C3	H3	124.7
C2	C3	H3	124.7	Ce1	C3	H3	110.2
C3	C4	C5	105.8(3)	C3	C4	C14	126.2(4)
C5	C4	C14	128.0(4)	C3	C4	Ce1	76.8(2)
C5	C4	Ce1	78.3(2)	C14	C4	Ce1	110.5(2)
C4	C5	C1	110.7(4)	C4	C5	Ce1	72.7(2)
C1	C5	Ce1	82.8(2)	C4	C5	H5	124.6
C1	C5	H5	124.6	Ce1	C5	H5	111.9
C9	C6	C7	105.9(3)	C9	C6	C8	106.0(3)
C7	C6	C8	110.3(3)	C9	C6	C1	111.2(3)
C7	C6	C1	109.5(3)	C8	C6	C1	113.7(3)
C6	C7	H7A	109.5	C6	C7	H7B	109.5
H7A	C7	H7B	109.5	C6	C7	H7C	109.5
H7A	C7	H7C	109.5	H7B	C7	H7C	109.5
C6	C8	H8A	109.5	C6	C8	H8B	109.5
H8A	C8	H8B	109.5	C6	C8	H8C	109.5
H8A	C8	H8C	109.5	H8B	C8	H8C	109.5
C6	C9	H9A	109.5	C6	C9	H9B	109.5
H9A	C9	H9B	109.5	C6	C9	H9C	109.5
H9A	C9	H9C	109.5	H9B	C9	H9C	109.5
C13	C10	C11	105.4(4)	C13	C10	C12	106.7(4)
C11	C10	C12	108.3(3)	C13	C10	C2	111.7(3)
C11	C10	C2	117.6(3)	C12	C10	C2	106.7(4)
C10	C11	H11A	109.5	C10	C11	H11B	109.5
H11A	C11	H11B	109.5	C10	C11	H11C	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5
C10	C12	H12A	109.5	C10	C12	H12B	109.5
H12A	C12	H12B	109.5	C10	C12	H12C	109.5
H12A	C12	H12C	109.5	H12B	C12	H12C	109.5
C10	C13	H13A	109.5	C10	C13	H13B	109.5
H13A	C13	H13B	109.5	C10	C13	H13C	109.5
H13A	C13	H13C	109.5	H13B	C13	H13C	109.5
C4	C14	C15	110.7(3)	C4	C14	C17	110.2(3)
C15	C14	C17	109.7(3)	C4	C14	C16	108.9(3)
C15	C14	C16	109.0(3)	C17	C14	C16	108.3(3)
C14	C15	H15A	109.5	C14	C15	H15B	109.5
H15A	C15	H15B	109.5	C14	C15	H15C	109.5

H15A	C15	H15C	109.5	H15B	C15	H15C	109.5
C14	C16	H16A	109.5	C14	C16	H16B	109.5
H16A	C16	H16B	109.5	C14	C16	H16C	109.5
H16A	C16	H16C	109.5	H16B	C16	H16C	109.5
C14	C17	H17A	109.5	C14	C17	H17B	109.5
H17A	C17	H17B	109.5	C14	C17	H17C	109.5
H17A	C17	H17C	109.5	H17B	C17	H17C	109.5
C22	C18	C19	105.4(4)	C22	C18	C23	117.8(4)
C19	C18	C23	134.4(4)	C22	C18	Ce1	68.6(2)
C19	C18	Ce1	76.7(2)	C23	C18	Ce1	131.5(3)
C20	C19	C18	106.8(3)	C20	C19	C27	121.5(4)
C18	C19	C27	130.9(4)	C20	C19	Ce1	69.7(2)
C18	C19	Ce1	75.1(2)	C27	C19	Ce1	127.9(3)
C21	C20	C19	110.8(4)	C21	C20	Ce1	73.4(2)
C19	C20	Ce1	82.0(2)	C21	C20	H20	124.6
C19	C20	H20	124.6	Ce1	C20	H20	112.0
C22	C21	C20	105.9(4)	C22	C21	C31	125.4(4)
C20	C21	C31	128.7(4)	C22	C21	Ce1	75.7(2)
C20	C21	Ce1	77.5(2)	C31	C21	Ce1	111.9(2)
C21	C22	C18	111.1(4)	C21	C22	Ce1	75.0(2)
C18	C22	Ce1	82.5(2)	C21	C22	H22	124.5
C18	C22	H22	124.5	Ce1	C22	H22	110.1
C24	C23	C26	105.2(4)	C24	C23	C25	106.7(4)
C26	C23	C25	110.1(4)	C24	C23	C18	110.7(4)
C26	C23	C18	117.1(4)	C25	C23	C18	106.6(4)
C23	C24	H24A	109.5	C23	C24	H24B	109.5
H24A	C24	H24B	109.5	C23	C24	H24C	109.5
H24A	C24	H24C	109.5	H24B	C24	H24C	109.5
C23	C25	H25A	109.5	C23	C25	H25B	109.5
H25A	C25	H25B	109.5	C23	C25	H25C	109.5
H25A	C25	H25C	109.5	H25B	C25	H25C	109.5
C23	C26	H26A	109.5	C23	C26	H26B	109.5
H26A	C26	H26B	109.5	C23	C26	H26C	109.5
H26A	C26	H26C	109.5	H26B	C26	H26C	109.5
C28	C27	C30	105.9(4)	C28	C27	C29	110.8(4)
C30	C27	C29	105.1(3)	C28	C27	C19	113.6(3)
C30	C27	C19	110.2(3)	C29	C27	C19	110.8(3)
C27	C28	H28A	109.5	C27	C28	H28B	109.5
H28A	C28	H28B	109.5	C27	C28	H28C	109.5
H28A	C28	H28C	109.5	H28B	C28	H28C	109.5
C27	C29	H29A	109.5	C27	C29	H29B	109.5
H29A	C29	H29B	109.5	C27	C29	H29C	109.5
H29A	C29	H29C	109.5	H29B	C29	H29C	109.5
C27	C30	H30A	109.5	C27	C30	H30B	109.5
H30A	C30	H30B	109.5	C27	C30	H30C	109.5
H30A	C30	H30C	109.5	H30B	C30	H30C	109.5

C34	C31	C33	109.6(4)	C34	C31	C21	111.4(4)
C33	C31	C21	107.9(4)	C34	C31	C32	109.8(4)
C33	C31	C32	108.3(4)	C21	C31	C32	109.8(4)
C31	C32	H32A	109.5	C31	C32	H32B	109.5
H32A	C32	H32B	109.5	C31	C32	H32C	109.5
H32A	C32	H32C	109.5	H32B	C32	H32C	109.5
C31	C33	H33A	109.5	C31	C33	H33B	109.5
H33A	C33	H33B	109.5	C31	C33	H33C	109.5
H33A	C33	H33C	109.5	H33B	C33	H33C	109.5
C31	C34	H34A	109.5	C31	C34	H34B	109.5
H34A	C34	H34B	109.5	C31	C34	H34C	109.5
H34A	C34	H34C	109.5	H34B	C34	H34C	109.5
C36	C35	Ce1	93.1(3)	C36	C35	H35A	113.1
Ce1	C35	H35A	113.1	C36	C35	H35B	113.1
Ce1	C35	H35B	113.1	H35A	C35	H35B	110.5
C41	C36	C37	114.9(4)	C41	C36	C35	121.8(4)
C37	C36	C35	123.1(4)	C41	C36	Ce1	86.4(3)
C37	C36	Ce1	124.1(3)	C35	C36	Ce1	58.6(2)
C38	C37	C36	121.4(5)	C38	C37	H37	119.3
C36	C37	H37	119.3	C37	C38	C39	121.6(5)
C37	C38	H38	119.2	C39	C38	H38	119.2
C40	C39	C38	118.3(5)	C40	C39	H39	120.9
C38	C39	H39	120.9	C39	C40	C41	121.0(5)
C39	C40	H40	119.5	C41	C40	H40	119.5
C40	C41	C36	122.7(5)	C40	C41	H41	118.6
C36	C41	H41	118.6	C43	C42	C46	106.1(3)
C43	C42	C51	134.8(3)	C46	C42	C51	117.7(3)
C43	C42	Ce2	77.3(2)	C46	C42	Ce2	70.7(2)
C51	C42	Ce2	126.3(3)	C44	C43	C42	107.1(3)
C44	C43	C47	120.8(4)	C42	C43	C47	131.7(4)
C44	C43	Ce2	70.4(2)	C42	C43	Ce2	74.2(2)
C47	C43	Ce2	126.5(3)	C45	C44	C43	110.5(4)
C45	C44	Ce2	73.6(2)	C43	C44	Ce2	81.0(2)
C45	C44	H44	124.8	C43	C44	H44	124.8
Ce2	C44	H44	112.6	C46	C45	C44	106.0(3)
C46	C45	C55	128.5(4)	C44	C45	C55	125.4(4)
C46	C45	Ce2	76.0(2)	C44	C45	Ce2	77.0(2)
C55	C45	Ce2	110.6(2)	C45	C46	C42	110.3(4)
C45	C46	Ce2	74.4(2)	C42	C46	Ce2	80.0(2)
C45	C46	H46	124.9	C42	C46	H46	124.9
Ce2	C46	H46	112.8	C48	C47	C49	111.5(4)
C48	C47	C50	106.9(4)	C49	C47	C50	104.4(4)
C48	C47	C43	113.3(3)	C49	C47	C43	110.0(3)
C50	C47	C43	110.4(3)	C47	C48	H48A	109.5
C47	C48	H48B	109.5	H48A	C48	H48B	109.5
C47	C48	H48C	109.5	H48A	C48	H48C	109.5

H48B	C48	H48C	109.5	C47	C49	H49A	109.5
C47	C49	H49B	109.5	H49A	C49	H49B	109.5
C47	C49	H49C	109.5	H49A	C49	H49C	109.5
H49B	C49	H49C	109.5	C47	C50	H50A	109.5
C47	C50	H50B	109.5	H50A	C50	H50B	109.5
C47	C50	H50C	109.5	H50A	C50	H50C	109.5
H50B	C50	H50C	109.5	C54	C51	C53	106.2(4)
C54	C51	C52	107.5(4)	C53	C51	C52	107.2(3)
C54	C51	C42	111.1(3)	C53	C51	C42	117.2(3)
C52	C51	C42	107.2(3)	C51	C52	H52A	109.5
C51	C52	H52B	109.5	H52A	C52	H52B	109.5
C51	C52	H52C	109.5	H52A	C52	H52C	109.5
H52B	C52	H52C	109.5	C51	C53	H53A	109.5
C51	C53	H53B	109.5	H53A	C53	H53B	109.5
C51	C53	H53C	109.5	H53A	C53	H53C	109.5
H53B	C53	H53C	109.5	C51	C54	H54A	109.5
C51	C54	H54B	109.5	H54A	C54	H54B	109.5
C51	C54	H54C	109.5	H54A	C54	H54C	109.5
H54B	C54	H54C	109.5	C45	C55	C58	110.3(3)
C45	C55	C57	110.4(3)	C58	C55	C57	109.2(3)
C45	C55	C56	110.9(3)	C58	C55	C56	108.1(4)
C57	C55	C56	107.9(4)	C55	C56	H56A	109.5
C55	C56	H56B	109.5	H56A	C56	H56B	109.5
C55	C56	H56C	109.5	H56A	C56	H56C	109.5
H56B	C56	H56C	109.5	C55	C57	H57A	109.5
C55	C57	H57B	109.5	H57A	C57	H57B	109.5
C55	C57	H57C	109.5	H57A	C57	H57C	109.5
H57B	C57	H57C	109.5	C55	C58	H58A	109.5
C55	C58	H58B	109.5	H58A	C58	H58B	109.5
C55	C58	H58C	109.5	H58A	C58	H58C	109.5
H58B	C58	H58C	109.5	C63	C59	C60	106.1(3)
C63	C59	C64	120.4(4)	C60	C59	C64	133.1(4)
C63	C59	Ce2	70.5(2)	C60	C59	Ce2	75.0(2)
C64	C59	Ce2	124.4(3)	C61	C60	C59	106.7(3)
C61	C60	C68	118.8(3)	C59	C60	C68	133.2(3)
C61	C60	Ce2	70.7(2)	C59	C60	Ce2	76.4(2)
C68	C60	Ce2	127.3(3)	C62	C61	C60	110.6(4)
C62	C61	Ce2	74.7(2)	C60	C61	Ce2	80.3(2)
C62	C61	H61	124.7	C60	C61	H61	124.7
Ce2	C61	H61	112.3	C63	C62	C61	105.2(4)
C63	C62	C72	127.2(4)	C61	C62	C72	127.3(4)
C63	C62	Ce2	76.3(2)	C61	C62	Ce2	75.6(2)
C72	C62	Ce2	108.8(2)	C62	C63	C59	111.3(4)
C62	C63	Ce2	74.4(2)	C59	C63	Ce2	80.6(2)
C62	C63	H63	124.3	C59	C63	H63	124.3
Ce2	C63	H63	112.5	C65	C64	C66	106.6(4)

C65	C64	C59	111.3(3)	C66	C64	C59	112.7(3)
C65	C64	C67	104.8(3)	C66	C64	C67	110.0(4)
C59	C64	C67	111.1(3)	C64	C65	H65A	109.5
C64	C65	H65B	109.5	H65A	C65	H65B	109.5
C64	C65	H65C	109.5	H65A	C65	H65C	109.5
H65B	C65	H65C	109.5	C64	C66	H66A	109.5
C64	C66	H66B	109.5	H66A	C66	H66B	109.5
C64	C66	H66C	109.5	H66A	C66	H66C	109.5
H66B	C66	H66C	109.5	C64	C67	H67A	109.5
C64	C67	H67B	109.5	H67A	C67	H67B	109.5
C64	C67	H67C	109.5	H67A	C67	H67C	109.5
H67B	C67	H67C	109.5	C69	C68	C71	105.0(3)
C69	C68	C70	109.5(3)	C71	C68	C70	107.3(3)
C69	C68	C60	117.0(3)	C71	C68	C60	111.4(3)
C70	C68	C60	106.4(3)	C68	C69	H69A	109.5
C68	C69	H69B	109.5	H69A	C69	H69B	109.5
C68	C69	H69C	109.5	H69A	C69	H69C	109.5
H69B	C69	H69C	109.5	C68	C70	H70A	109.5
C68	C70	H70B	109.5	H70A	C70	H70B	109.5
C68	C70	H70C	109.5	H70A	C70	H70C	109.5
H70B	C70	H70C	109.5	C68	C71	H71A	109.5
C68	C71	H71B	109.5	H71A	C71	H71B	109.5
C68	C71	H71C	109.5	H71A	C71	H71C	109.5
H71B	C71	H71C	109.5	C62	C72	C74	108.7(3)
C62	C72	C75	110.8(4)	C74	C72	C75	108.8(4)
C62	C72	C73	110.8(4)	C74	C72	C73	108.5(4)
C75	C72	C73	109.2(4)	C72	C73	H73A	109.5
C72	C73	H73B	109.5	H73A	C73	H73B	109.5
C72	C73	H73C	109.5	H73A	C73	H73C	109.5
H73B	C73	H73C	109.5	C72	C74	H74A	109.5
C72	C74	H74B	109.5	H74A	C74	H74B	109.5
C72	C74	H74C	109.5	H74A	C74	H74C	109.5
H74B	C74	H74C	109.5	C72	C75	H75A	109.5
C72	C75	H75B	109.5	H75A	C75	H75B	109.5
C72	C75	H75C	109.5	H75A	C75	H75C	109.5
H75B	C75	H75C	109.5	C77	C76	Ce2	130.4(3)
C77	C76	H76A	104.7	Ce2	C76	H76A	104.7
C77	C76	H76B	104.7	Ce2	C76	H76B	104.7
H76A	C76	H76B	105.7	C78	C77	C82	115.7(4)
C78	C77	C76	122.8(4)	C82	C77	C76	121.5(4)
C79	C78	C77	121.5(4)	C79	C78	H78	119.2
C77	C78	H78	119.2	C80	C79	C78	120.5(4)
C80	C79	H79	119.7	C78	C79	H79	119.7
C79	C80	C81	119.3(4)	C79	C80	H80	120.4
C81	C80	H80	120.4	C82	C81	C80	119.9(4)
C82	C81	H81	120.0	C80	C81	H81	120.0

C81	C82	C77	123.0(4)	C81	C82	H82	118.5
C77	C82	H82	118.5	C35	Ce1	C21	93.93(14)
C35	Ce1	C4	114.99(13)	C21	Ce1	C4	147.85(12)
C35	Ce1	C22	123.15(14)	C21	Ce1	C22	29.26(12)
C4	Ce1	C22	119.87(13)	C35	Ce1	C3	132.33(13)
C21	Ce1	C3	119.58(12)	C4	Ce1	C3	29.14(11)
C22	Ce1	C3	94.14(12)	C35	Ce1	C20	85.12(13)
C21	Ce1	C20	29.16(11)	C4	Ce1	C20	156.15(12)
C22	Ce1	C20	47.19(12)	C3	Ce1	C20	140.20(12)
C35	Ce1	C5	88.15(13)	C21	Ce1	C5	154.07(11)
C4	Ce1	C5	29.03(11)	C22	Ce1	C5	139.42(12)
C3	Ce1	C5	46.80(12)	C20	Ce1	C5	173.00(12)
C35	Ce1	C18	131.82(13)	C21	Ce1	C18	48.22(12)
C4	Ce1	C18	110.93(12)	C22	Ce1	C18	28.94(11)
C3	Ce1	C18	95.40(12)	C20	Ce1	C18	46.98(12)
C5	Ce1	C18	139.46(11)	C35	Ce1	C19	106.13(13)
C21	Ce1	C19	47.72(11)	C4	Ce1	C19	128.09(11)
C22	Ce1	C19	46.92(11)	C3	Ce1	C19	121.42(11)
C20	Ce1	C19	28.30(11)	C5	Ce1	C19	154.78(11)
C18	Ce1	C19	28.22(11)	C35	Ce1	C2	111.91(12)
C21	Ce1	C2	110.16(12)	C4	Ce1	C2	47.48(11)
C22	Ce1	C2	94.91(12)	C3	Ce1	C2	28.31(10)
C20	Ce1	C2	138.95(11)	C5	Ce1	C2	46.16(11)
C18	Ce1	C2	109.32(11)	C19	Ce1	C2	137.46(11)
C35	Ce1	C1	87.09(12)	C21	Ce1	C1	126.35(11)
C4	Ce1	C1	47.21(11)	C22	Ce1	C1	120.15(12)
C3	Ce1	C1	46.29(11)	C20	Ce1	C1	152.96(11)
C5	Ce1	C1	27.86(11)	C18	Ce1	C1	137.03(11)
C19	Ce1	C1	165.20(11)	C2	Ce1	C1	27.75(10)
C35	Ce1	C36	28.29(12)	C21	Ce1	C36	103.34(12)
C4	Ce1	C36	108.80(12)	C22	Ce1	C36	129.44(13)
C3	Ce1	C36	136.32(12)	C20	Ce1	C36	82.53(12)
C5	Ce1	C36	90.62(12)	C18	Ce1	C36	120.80(11)
C19	Ce1	C36	92.64(11)	C2	Ce1	C36	129.88(11)
C1	Ce1	C36	102.15(11)	C76	Ce2	C45	91.34(13)
C76	Ce2	C62	100.79(13)	C45	Ce2	C62	167.71(12)
C76	Ce2	C46	79.65(13)	C45	Ce2	C46	29.56(11)
C62	Ce2	C46	151.19(12)	C76	Ce2	C61	81.47(13)
C45	Ce2	C61	158.28(11)	C62	Ce2	C61	29.66(11)
C46	Ce2	C61	159.98(12)	C76	Ce2	C63	128.02(13)
C45	Ce2	C63	139.55(12)	C62	Ce2	C63	29.33(12)
C46	Ce2	C63	148.34(12)	C61	Ce2	C63	47.56(12)
C76	Ce2	C44	120.71(13)	C45	Ce2	C44	29.43(11)
C62	Ce2	C44	138.33(12)	C46	Ce2	C44	47.71(12)
C61	Ce2	C44	151.83(12)	C63	Ce2	C44	110.85(12)
C76	Ce2	C42	100.20(12)	C45	Ce2	C42	48.85(11)

C62	Ce2	C42	125.69(11)	C46	Ce2	C42	29.34(11)
C61	Ce2	C42	152.56(11)	C63	Ce2	C42	120.01(11)
C44	Ce2	C42	47.61(12)	C76	Ce2	C60	94.22(13)
C45	Ce2	C60	133.00(11)	C62	Ce2	C60	48.70(11)
C46	Ce2	C60	159.81(11)	C61	Ce2	C60	28.99(11)
C63	Ce2	C60	47.43(11)	C44	Ce2	C60	124.86(11)
C42	Ce2	C60	165.48(11)	C76	Ce2	C59	122.81(13)
C45	Ce2	C59	125.41(11)	C62	Ce2	C59	48.54(11)
C46	Ce2	C59	152.13(12)	C61	Ce2	C59	47.52(11)
C63	Ce2	C59	28.87(11)	C44	Ce2	C59	104.47(11)
C42	Ce2	C59	136.89(11)	C60	Ce2	C59	28.62(11)
C76	Ce2	C43	126.35(13)	C45	Ce2	C43	48.19(11)
C62	Ce2	C43	120.91(12)	C46	Ce2	C43	47.39(11)
C61	Ce2	C43	148.91(11)	C63	Ce2	C43	101.93(12)
C44	Ce2	C43	28.63(11)	C42	Ce2	C43	28.51(11)
C60	Ce2	C43	138.17(11)	C59	Ce2	C43	110.29(11)

1.5 Least Squares Planes for $Cp'_2CeCH_2C_6H_5$

Plane number 1

Atoms defining plane	Distance
C(1)	0.0034(24)
C(2)	0.0058(24)
C(3)	-0.0128(24)
C(4)	0.0148(24)
C(5)	-0.0112(24)

Additional Atoms	Distance
C(6)	0.2432(68)
C(10)	0.4138(70)
C(14)	0.0514(67)

Plane number 2

Atoms defining plane	Distance
C(18)	0.0054(25)
C(19)	0.0067(25)
C(20)	-0.0162(25)

C(21)	0.0196(25)
C(22)	0.0154(26)

Additional Atoms	Distance
C(23)	0.3825(76)
C(27)	0.2407(71)
C(31)	0.0645(72)

Plane number 3

Atoms defining plane	Distance
C(42)	-0.0086(25)
C(43)	0.0149(25)
C(44)	-0.0156(25)
C(45)	0.0099(25)
C(46)	-0.0006(25)

Additional Atoms	Distance
C(47)	0.2297(70)
C(51)	0.2350(71)
C(55)	0.0175(70)

Plane number 4

Atoms defining plane	Distance
C(59)	-0.0071(24)
C(60)	-0.0009(24)
C(61)	0.0084(25)
C(62)	-0.0129(25)
C(63)	0.0125(25)

Additional Atoms	Distance
C(64)	-0.1746(71)
C(68)	-0.2687(71)
C(72)	0.0724(72)

Plane number 5

Atoms defining plane	Distance
C(36)	-0.0072(31)
C(37)	0.0114(33)
C(38)	-0.0074(36)
C(39)	-0.0010(37)
C(40)	0.0050(36)
C(41)	-0.0008(33)

Additional Atoms	Distance
C(35)	0.0670(69)

Plane number 6

Atoms defining plane	Distance
Ce(1)	0.0
C(35)	0.0
C(36)	0.0

Plane number 7

Atoms defining plane	Distance
C(77)	-0.0003(28)
C(78)	0.0015(30)
C(79)	0.0000(33)
C(80)	-0.0026(33)
C(81)	0.0039(32)
C(82)	-0.0024(30)

Additional Atoms	Distance
C(76)	-0.0185(67)

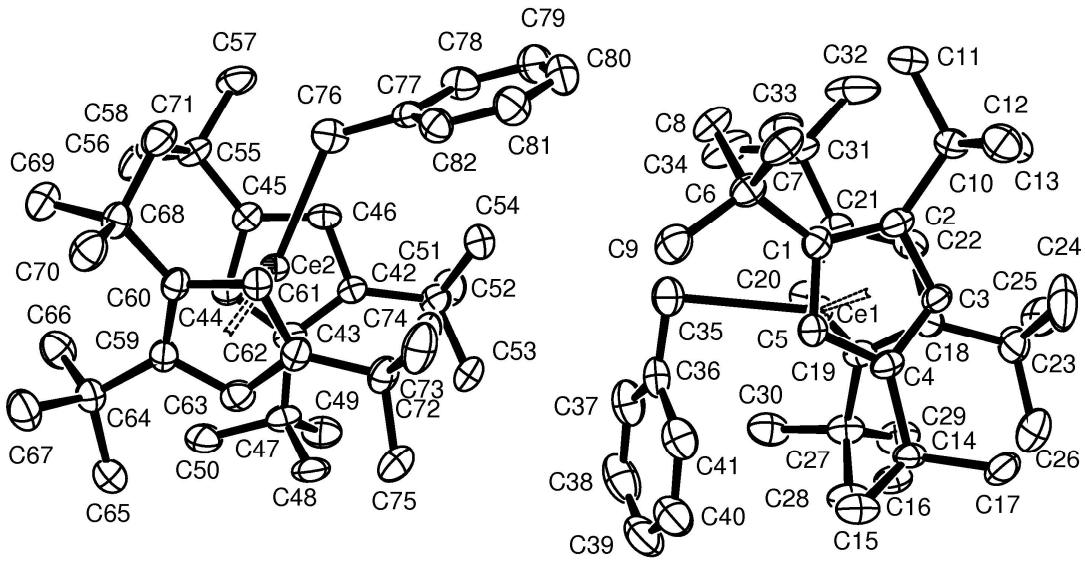
Plane number 8

Atoms defining plane	Distance
Ce(2)	0.0
C(76)	0.0
C(77)	0.0

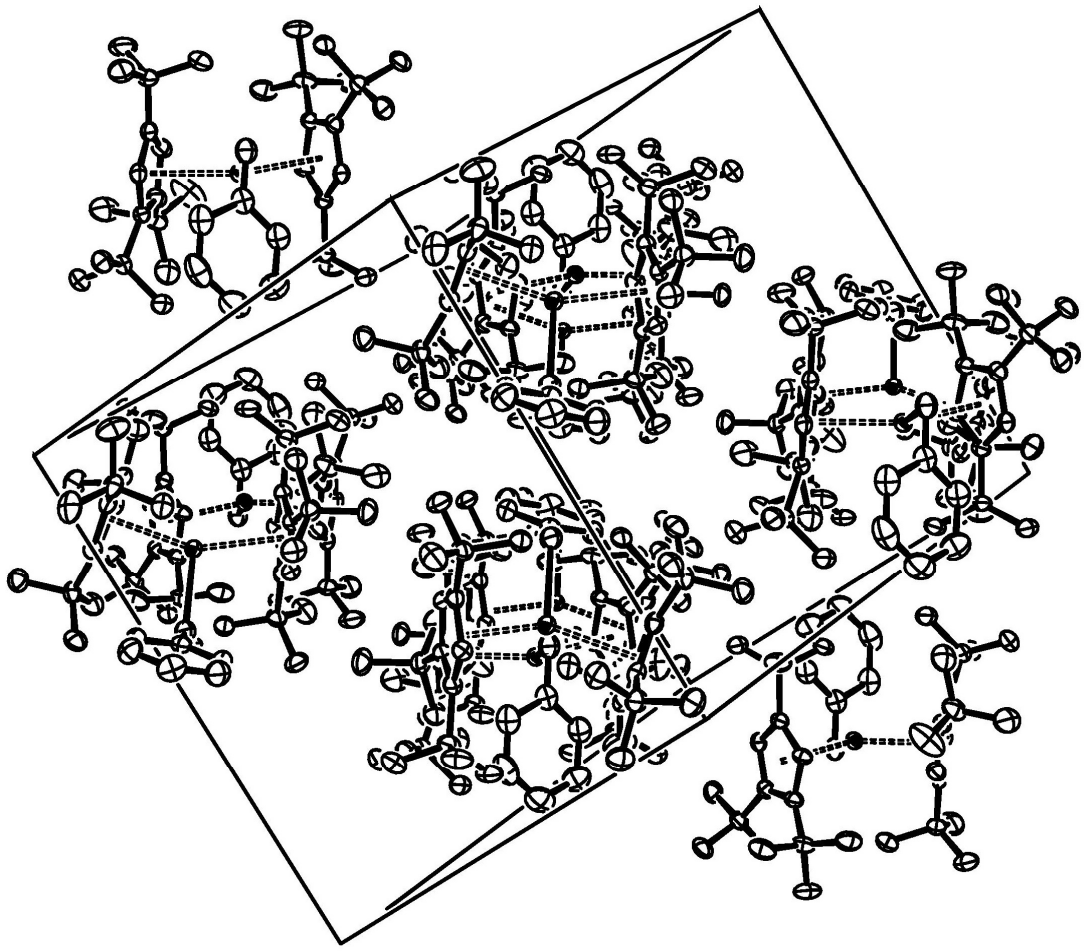
Dihedral angles between planes (^{o})

plane	1	2	3	4	5	6	7
2	41.99						
3		25.85					
4			26.67				
5				61.70			
6					64.49		
7						81.44	
8							79.48

1.6 ORTEP (50% ellipsoids) showing atom labeling scheme for $Cp'_2CeCH_2C_6H_5$



1.7 Packing diagram for $Cp'_2CeCH_2C_6H_5$



2. Cp'$_2$Ce[4-methylbenzyl] • 0.5(pentane)

Data Collection

A fragment of a red block-like crystal of [1,2,4-$(Me_3C)_3C_5H_2]_2$Ce-4-methylbenzyl having approximate dimensions of 0.26 x 0.12 x 0.07 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker SMART 1000 CCD [10] area detector with graphite monochromated MoKα radiation. Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 6536 centered reflections with $I > 10\sigma(I)$ in the range $5.878 < \theta < 50.594^o$ corresponded to a primitive triclinic cell with dimensions:

a = 10.528(2) Å	α = 84.069(4) ^{o}
b = 12.032(3) Å	β = 79.816(4) ^{o}
c = 17.562(4) Å	γ = 66.418(3) ^{o}
V = 2005.4(8) Å^3	

For Z = 2 and F.W. = 744.64, the calculated density is 1.233 g/cm^3. Analysis of the systematic absences allowed the space group to be uniquely determined to be $P\bar{1}$ (#2).

The data were collected at a temperature of 120(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ϕ and ω scans of 0.3^o counted for a total of 10 seconds per frame.

Data were integrated by the program SAINT[11] to a maximum θ value of 25.47^o. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[13]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[12]. (Tmax = 0.8786, Tmin = 0.7900). Of the 18167 reflections that were collected, 7273 were unique (R_{int} = 0.0821); equivalent reflections were merged. No decay correction was applied.

The structure was solved by direct methods[14] and expanded using Fourier techniques[15]. Non-hydrogen atoms in the organometallic molecule were refined anisotropically. The asymmetric unit was found to contain half a molecule of pentane disordered about the inversion center. This was modeled using four carbon atoms with an occupancy of 0.5 (C43, C44, C46, C47) and the central carbon atom on the inversion center (C45) with an occupancy of 0.25. Hydrogen atoms were included in calculated positions but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 7273 reflections (all data) and 424 variable parameters and converged (largest parameter shift was 0.000 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0493 \text{ for 4054 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.0933$$

The standard deviation of an observation of unit weight[4] was 0.843. The weighting scheme was based on counting statistics and included a factor (q = 0.0573) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.506 and -1.290 e$^-$/Å^3, respectively, located in the vicinity of the cerium atom.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[16] crystallographic software package of Bruker Analytical X-ray Systems Inc.

2.1 Atomic coordinates and B_{iso}/B_{eq} for Cp'$_2$Ce[4-methylbenzyl] •

0.5(pentane)

atom	x	y	z	U_{eq}	Occupancy
C1	0.3420(7)	0.3102(7)	0.0990(4)	0.026(2)	1
C2	0.3603(7)	0.3720(6)	0.1568(4)	0.022(2)	1
C3	0.5030(7)	0.3541(6)	0.1519(4)	0.018(2)	1
C4	0.5774(7)	0.2747(7)	0.0901(4)	0.022(2)	1
C5	0.4790(7)	0.2456(6)	0.0602(4)	0.024(2)	1
C6	0.2061(7)	0.3136(7)	0.0791(4)	0.024(2)	1
C7	0.1877(8)	0.1957(8)	0.1126(6)	0.061(3)	1
C8	0.2084(8)	0.3248(8)	-0.0076(5)	0.046(3)	1
C9	0.0795(7)	0.4216(7)	0.1150(5)	0.037(2)	1
C10	0.5353(7)	0.4440(6)	0.1952(4)	0.025(2)	1
C11	0.6873(8)	0.4035(7)	0.2116(5)	0.038(2)	1
C12	0.4442(8)	0.4704(8)	0.2746(5)	0.043(2)	1
C13	0.4969(9)	0.5632(7)	0.1471(5)	0.046(3)	1
C14	0.7271(7)	0.2388(7)	0.0441(5)	0.031(2)	1
C15	0.8425(7)	0.1646(7)	0.0957(5)	0.035(2)	1
C16	0.7469(8)	0.1616(7)	-0.0250(4)	0.037(2)	1
C17	0.7536(8)	0.3503(7)	0.0090(5)	0.038(2)	1
C18	0.4784(7)	0.0814(7)	0.3641(4)	0.031(2)	1
C19	0.4341(7)	-0.0072(7)	0.3470(4)	0.029(2)	1
C20	0.2881(7)	0.0496(7)	0.3373(4)	0.022(2)	1
C21	0.2448(7)	0.1753(6)	0.3496(4)	0.020(2)	1
C22	0.3639(7)	0.1917(6)	0.3638(4)	0.020(2)	1
C23	0.6249(7)	0.0613(7)	0.3763(4)	0.026(2)	1
C24	0.6182(7)	0.1511(7)	0.4348(5)	0.043(2)	1
C25	0.7093(7)	0.0838(8)	0.2985(4)	0.038(2)	1
C26	0.7017(8)	-0.0664(7)	0.4091(5)	0.044(2)	1
C27	0.2058(7)	-0.0332(7)	0.3336(5)	0.029(2)	1
C28	0.3025(8)	-0.1654(7)	0.3280(5)	0.044(2)	1
C29	0.1286(7)	0.0010(7)	0.2586(4)	0.030(2)	1
C30	0.0984(8)	-0.0220(7)	0.4065(5)	0.035(2)	1
C31	0.0986(7)	0.2794(6)	0.3699(5)	0.026(2)	1
C32	-0.0219(8)	0.2834(8)	0.3299(5)	0.047(3)	1
C33	0.1096(8)	0.4045(6)	0.3504(5)	0.035(2)	1
C34	0.0541(8)	0.2758(7)	0.4572(5)	0.041(2)	1
C35	0.4928(7)	-0.0588(6)	0.1396(4)	0.027(2)	1
C36	0.6272(7)	-0.1216(6)	0.1601(4)	0.026(2)	1
C37	0.6656(7)	-0.2232(6)	0.2146(4)	0.025(2)	1
C38	0.8002(7)	-0.2802(7)	0.2348(5)	0.032(2)	1
C39	0.9048(8)	-0.2365(7)	0.2041(5)	0.030(2)	1
C40	0.8682(8)	-0.1360(8)	0.1512(5)	0.040(2)	1
C41	0.7386(8)	-0.0869(7)	0.1345(4)	0.030(2)	1

C42	1.0468(8)	-0.2977(7)	0.2271(6)	0.050(3)	1
C43	0.3031(18)	0.4181(16)	0.5401(11)	0.038(5)	0.50
C44	0.384(2)	0.485(2)	0.5022(15)	0.079(7)	0.50
C45	0.5000	0.5000	0.5000	0.016(5)	0.50
C46	0.562(3)	0.551(2)	0.4505(15)	0.091(8)	0.50
C47	0.647(2)	0.590(2)	0.4322(13)	0.066(7)	0.50
Ce1	0.4597(1)	0.1310(1)	0.2095(1)	0.023(1)	1
H2	0.2869	0.4196	0.1943	0.026	1
H5	0.5013	0.1909	0.0199	0.028	1
H7A	0.0922	0.2036	0.1102	0.092	1
H7B	0.2045	0.1821	0.1666	0.092	1
H7C	0.2550	0.1269	0.0823	0.092	1
H8A	0.2204	0.3996	-0.0276	0.070	1
H8B	0.1198	0.3272	-0.0196	0.070	1
H8C	0.2863	0.2549	-0.0318	0.070	1
H9A	0.0835	0.4973	0.0906	0.056	1
H9B	0.0812	0.4211	0.1707	0.056	1
H9C	-0.0071	0.4154	0.1068	0.056	1
H11A	0.7504	0.3974	0.1625	0.057	1
H11B	0.7152	0.3243	0.2391	0.057	1
H11C	0.6927	0.4633	0.2435	0.057	1
H12A	0.4703	0.3964	0.3077	0.064	1
H12B	0.3453	0.4981	0.2685	0.064	1
H12C	0.4585	0.5338	0.2986	0.064	1
H13A	0.5202	0.6209	0.1715	0.069	1
H13B	0.3963	0.5971	0.1443	0.069	1
H13C	0.5497	0.5479	0.0948	0.069	1
H15A	0.8270	0.0922	0.1180	0.052	1
H15B	0.8376	0.2150	0.1374	0.052	1
H15C	0.9351	0.1402	0.0640	0.052	1
H16A	0.8402	0.1442	-0.0550	0.056	1
H16B	0.6753	0.2062	-0.0581	0.056	1
H16C	0.7379	0.0852	-0.0060	0.056	1
H17A	0.7531	0.3991	0.0505	0.057	1
H17B	0.6799	0.3990	-0.0220	0.057	1
H17C	0.8449	0.3246	-0.0242	0.057	1
H19	0.4909	-0.0913	0.3426	0.034	1
H22	0.3657	0.2679	0.3721	0.024	1
H24A	0.5826	0.2338	0.4123	0.064	1
H24B	0.7123	0.1309	0.4473	0.064	1
H24C	0.5555	0.1457	0.4822	0.064	1
H25A	0.7252	0.0210	0.2624	0.057	1
H25B	0.7997	0.0808	0.3079	0.057	1
H25C	0.6563	0.1638	0.2762	0.057	1
H26A	0.6467	-0.0804	0.4575	0.066	1
H26B	0.7937	-0.0746	0.4192	0.066	1

H26C	0.7139	-0.1262	0.3716	0.066	1
H28A	0.3729	-0.1762	0.2816	0.066	1
H28B	0.2481	-0.2140	0.3246	0.066	1
H28C	0.3493	-0.1919	0.3740	0.066	1
H29A	0.1986	-0.0133	0.2119	0.045	1
H29B	0.0650	0.0868	0.2593	0.045	1
H29C	0.0749	-0.0493	0.2588	0.045	1
H30A	0.0655	-0.0881	0.4095	0.052	1
H30B	0.0188	0.0561	0.4044	0.052	1
H30C	0.1421	-0.0268	0.4522	0.052	1
H32A	-0.1081	0.3515	0.3488	0.071	1
H32B	-0.0360	0.2073	0.3415	0.071	1
H32C	0.0015	0.2939	0.2738	0.071	1
H33A	0.0153	0.4684	0.3527	0.052	1
H33B	0.1615	0.4042	0.2982	0.052	1
H33C	0.1590	0.4196	0.3880	0.052	1
H34A	0.1115	0.3032	0.4829	0.061	1
H34B	0.0672	0.1926	0.4751	0.061	1
H34C	-0.0448	0.3294	0.4699	0.061	1
H35A	0.4256	-0.0961	0.1625	0.033	1
H35B	0.4930	-0.0449	0.0830	0.033	1
H37	0.5961	-0.2529	0.2380	0.030	1
H38	0.8212	-0.3490	0.2696	0.039	1
H40	0.9356	-0.1039	0.1280	0.048	1
H41	0.7193	-0.0180	0.0999	0.037	1
H42A	1.1056	-0.2540	0.2031	0.075	1
H42B	1.0892	-0.3814	0.2099	0.075	1
H42C	1.0391	-0.2980	0.2836	0.075	1
H10A	0.2146	0.4456	0.5193	0.056	0.50
H10B	0.2835	0.4316	0.5959	0.056	0.50
H10C	0.3560	0.3315	0.5312	0.056	0.50
H10D	0.3889	0.4694	0.4472	0.095	0.50
H10E	0.3142	0.5695	0.5088	0.095	0.50
H10F	0.4874	0.5404	0.5487	0.019	0.25
H10G	0.5710	0.4169	0.5063	0.019	0.25
H10H	0.5848	0.4969	0.4070	0.109	0.50
H10I	0.4794	0.6231	0.4374	0.109	0.50
H10J	0.6459	0.6198	0.3782	0.099	0.50
H10K	0.7392	0.5260	0.4376	0.099	0.50
H10L	0.6292	0.6569	0.4654	0.099	0.50

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

2.2 Anisotropic Displacement Parameters for Cp'$_2$Ce[4-methylbenzyl] ●

0.5(pentane)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.019(4)	0.039(5)	0.027(5)	-0.005(4)	-0.005(3)	-0.016(4)
C2	0.020(4)	0.029(5)	0.013(4)	0.001(4)	-0.004(3)	-0.007(3)
C3	0.020(4)	0.011(4)	0.024(5)	0.011(3)	-0.015(3)	-0.005(3)
C4	0.018(4)	0.027(5)	0.024(5)	0.005(4)	-0.009(3)	-0.011(3)
C5	0.018(4)	0.028(5)	0.028(5)	-0.009(4)	0.001(3)	-0.011(3)
C6	0.019(4)	0.033(5)	0.025(5)	0.009(4)	-0.014(3)	-0.013(4)
C7	0.030(5)	0.047(6)	0.121(10)	0.038(6)	-0.040(6)	-0.027(5)
C8	0.033(5)	0.077(7)	0.032(6)	-0.021(5)	-0.005(4)	-0.019(5)
C9	0.026(4)	0.046(6)	0.036(6)	0.009(5)	-0.007(4)	-0.012(4)
C10	0.030(4)	0.018(4)	0.030(5)	0.002(4)	-0.013(4)	-0.010(4)
C11	0.041(5)	0.035(5)	0.051(6)	-0.004(5)	-0.025(4)	-0.021(4)
C12	0.046(5)	0.049(6)	0.043(6)	-0.027(5)	-0.001(4)	-0.024(5)
C13	0.044(5)	0.047(6)	0.058(7)	-0.020(5)	-0.003(5)	-0.029(5)
C14	0.018(4)	0.048(6)	0.032(5)	-0.006(4)	0.008(4)	-0.021(4)
C15	0.017(4)	0.042(5)	0.045(6)	0.002(5)	-0.006(4)	-0.012(4)
C16	0.028(4)	0.059(6)	0.028(5)	-0.008(5)	0.012(4)	-0.025(4)
C17	0.032(5)	0.057(6)	0.037(6)	0.009(5)	-0.008(4)	-0.031(5)
C18	0.022(4)	0.055(6)	0.024(5)	-0.020(4)	0.010(4)	-0.024(4)
C19	0.019(4)	0.023(5)	0.040(6)	-0.002(4)	0.002(4)	-0.006(3)
C20	0.016(4)	0.038(5)	0.013(4)	0.003(4)	-0.005(3)	-0.011(4)
C21	0.017(4)	0.022(4)	0.018(5)	0.005(3)	0.000(3)	-0.005(3)
C22	0.018(4)	0.023(4)	0.016(4)	-0.003(4)	0.001(3)	-0.004(3)
C23	0.018(4)	0.032(5)	0.026(5)	-0.009(4)	-0.006(3)	-0.005(4)
C24	0.016(4)	0.061(6)	0.052(6)	-0.022(5)	-0.010(4)	-0.008(4)
C25	0.011(4)	0.065(6)	0.034(6)	0.007(5)	-0.007(4)	-0.011(4)
C26	0.022(4)	0.041(6)	0.071(7)	0.000(5)	-0.024(5)	-0.007(4)
C27	0.023(4)	0.028(5)	0.037(6)	0.015(4)	-0.013(4)	-0.011(4)
C28	0.027(5)	0.036(5)	0.074(7)	-0.004(5)	-0.003(5)	-0.019(4)
C29	0.021(4)	0.028(5)	0.046(6)	0.007(4)	-0.011(4)	-0.014(4)
C30	0.027(4)	0.036(5)	0.043(6)	0.025(4)	-0.010(4)	-0.018(4)
C31	0.009(4)	0.021(4)	0.037(5)	0.006(4)	-0.010(3)	0.008(3)
C32	0.022(4)	0.057(6)	0.064(7)	-0.024(5)	0.006(4)	-0.016(4)
C33	0.028(4)	0.021(5)	0.042(6)	-0.005(4)	-0.008(4)	0.006(4)
C34	0.030(5)	0.042(6)	0.037(6)	0.000(5)	0.005(4)	-0.005(4)
C35	0.025(4)	0.028(5)	0.027(5)	-0.001(4)	-0.008(4)	-0.006(4)
C36	0.025(4)	0.018(4)	0.030(5)	-0.008(4)	-0.004(4)	0.001(3)
C37	0.024(4)	0.010(4)	0.035(5)	0.009(4)	-0.014(4)	-0.001(3)
C38	0.027(4)	0.024(5)	0.039(6)	0.001(4)	-0.002(4)	-0.006(4)
C39	0.027(4)	0.015(4)	0.043(6)	-0.004(4)	-0.005(4)	-0.003(4)
C40	0.023(4)	0.046(6)	0.051(6)	-0.004(5)	0.008(4)	-0.019(4)
C41	0.038(5)	0.025(5)	0.028(5)	0.013(4)	-0.006(4)	-0.014(4)
C42	0.027(5)	0.032(5)	0.088(8)	-0.007(5)	-0.009(5)	-0.008(4)

Ce1	0.021(1)	0.026(1)	0.022(1)	-0.001(1)	-0.003(1)	-0.011(1)

The general temperature factor expression:

$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$

2.3. Bond Lengths (Å) for Cp'$_2$Ce[4-methylbenzyl] ● 0.5(pentane)

atom	atom	distance	atom	atom	distance
C1	C2	1.400(9)	C1	C5	1.419(9)
C1	C6	1.517(9)	C1	Ce1	2.792(8)
C2	C3	1.417(8)	C2	Ce1	2.778(7)
C2	H2	0.9500	C3	C4	1.421(9)
C3	C10	1.556(9)	C3	Ce1	2.948(6)
C4	C5	1.412(8)	C4	C14	1.550(9)
C4	Ce1	2.995(7)	C5	Ce1	2.848(8)
C5	H5	0.9500	C6	C8	1.512(10)
C6	C9	1.533(10)	C6	C7	1.550(10)
C7	H7A	0.9800	C7	H7B	0.9800
C7	H7C	0.9800	C8	H8A	0.9800
C8	H8B	0.9800	C8	H8C	0.9800
C9	H9A	0.9800	C9	H9B	0.9800
C9	H9C	0.9800	C10	C13	1.529(11)
C10	C12	1.531(10)	C10	C11	1.546(9)
C11	H11A	0.9800	C11	H11B	0.9800
C11	H11C	0.9800	C12	H12A	0.9800
C12	H12B	0.9800	C12	H12C	0.9800
C13	H13A	0.9800	C13	H13B	0.9800
C13	H13C	0.9800	C14	C17	1.525(10)
C14	C16	1.539(10)	C14	C15	1.564(10)
C15	H15A	0.9800	C15	H15B	0.9800
C15	H15C	0.9800	C16	H16A	0.9800
C16	H16B	0.9800	C16	H16C	0.9800
C17	H17A	0.9800	C17	H17B	0.9800
C17	H17C	0.9800	C18	C22	1.392(10)
C18	C19	1.399(9)	C18	C23	1.513(9)
C18	Ce1	2.743(8)	C19	C20	1.444(9)
C19	Ce1	2.823(8)	C19	H19	0.9500
C20	C21	1.423(9)	C20	C27	1.573(9)
C20	Ce1	2.964(7)	C21	C22	1.412(8)
C21	C31	1.556(9)	C21	Ce1	2.965(6)
C22	Ce1	2.784(7)	C22	H22	0.9500
C23	C26	1.528(10)	C23	C24	1.541(9)
C23	C25	1.554(10)	C24	H24A	0.9800
C24	H24B	0.9800	C24	H24C	0.9800

C25	H25A	0.9800	C25	H25B	0.9800
C25	H25C	0.9800	C26	H26A	0.9800
C26	H26B	0.9800	C26	H26C	0.9800
C27	C28	1.509(10)	C27	C30	1.528(10)
C27	C29	1.601(10)	C28	H28A	0.9800
C28	H28B	0.9800	C28	H28C	0.9800
C29	H29A	0.9800	C29	H29B	0.9800
C29	H29C	0.9800	C30	H30A	0.9800
C30	H30B	0.9800	C30	H30C	0.9800
C31	C34	1.524(10)	C31	C32	1.539(10)
C31	C33	1.553(9)	C32	H32A	0.9800
C32	H32B	0.9800	C32	H32C	0.9800
C33	H33A	0.9800	C33	H33B	0.9800
C33	H33C	0.9800	C34	H34A	0.9800
C34	H34B	0.9800	C34	H34C	0.9800
C35	C36	1.404(9)	C35	Ce1	2.576(7)
C35	H35A	0.9900	C35	H35B	0.9900
C36	C41	1.385(9)	C36	C37	1.441(10)
C36	Ce1	2.969(7)	C37	C38	1.398(9)
C37	H37	0.9500	C38	C39	1.406(10)
C38	H38	0.9500	C39	C40	1.412(11)
C39	C42	1.488(10)	C40	C41	1.327(10)
C40	H40	0.9500	C41	H41	0.9500
C42	H42A	0.9800	C42	H42B	0.9800
C42	H42C	0.9800	C43	C44	1.43(3)
C43	H10A	0.9800	C43	H10B	0.9800
C43	H10C	0.9800	C44	C45	1.30(2)
C44	H10D	0.9900	C44	H10E	0.9900
C45	C46	1.25(2)	C45	H10F	0.9900
C45	H10G	0.9900	C46	C47	1.16(2)
C46	H10H	0.9900	C46	H10I	0.9900
C47	H10J	0.9800	C47	H10K	0.9800
C47	H10L	0.9800			

2.4. Bond Angles(°) for Cp'$_2$Ce[4-methylbenzyl] • 0.5(pentane)

atom	atom	atom	angle	atom	atom	atom	angle
C2	C1	C5	105.2(6)	C2	C1	C6	128.2(6)
C5	C1	C6	126.5(6)	C2	C1	Ce1	74.9(4)
C5	C1	Ce1	77.6(5)	C6	C1	Ce1	114.7(5)
C1	C2	C3	111.0(6)	C1	C2	Ce1	76.0(4)
C3	C2	Ce1	82.4(4)	C1	C2	H2	124.5
C3	C2	H2	124.5	Ce1	C2	H2	109.3
C2	C3	C4	106.3(6)	C2	C3	C10	117.1(6)
C4	C3	C10	134.1(6)	C2	C3	Ce1	69.1(4)

C4	C3	Ce1	78.0(4)	C10	C3	Ce1	130.1(5)
C5	C4	C3	107.3(6)	C5	C4	C14	118.5(6)
C3	C4	C14	133.0(6)	C5	C4	Ce1	70.3(4)
C3	C4	Ce1	74.3(4)	C14	C4	Ce1	129.7(5)
C4	C5	C1	110.0(6)	C4	C5	Ce1	81.9(4)
C1	C5	Ce1	73.2(4)	C4	C5	H5	125.0
C1	C5	H5	125.0	Ce1	C5	H5	112.0
C8	C6	C1	110.4(6)	C8	C6	C9	107.9(7)
C1	C6	C9	111.5(6)	C8	C6	C7	110.8(7)
C1	C6	C7	108.3(6)	C9	C6	C7	107.9(6)
C6	C7	H7A	109.5	C6	C7	H7B	109.5
H7A	C7	H7B	109.5	C6	C7	H7C	109.5
H7A	C7	H7C	109.5	H7B	C7	H7C	109.5
C6	C8	H8A	109.5	C6	C8	H8B	109.5
H8A	C8	H8B	109.5	C6	C8	H8C	109.5
H8A	C8	H8C	109.5	H8B	C8	H8C	109.5
C6	C9	H9A	109.5	C6	C9	H9B	109.5
H9A	C9	H9B	109.5	C6	C9	H9C	109.5
H9A	C9	H9C	109.5	H9B	C9	H9C	109.5
C13	C10	C12	107.8(6)	C13	C10	C11	108.9(6)
C12	C10	C11	105.0(6)	C13	C10	C3	107.2(6)
C12	C10	C3	110.7(6)	C11	C10	C3	116.9(6)
C10	C11	H11A	109.5	C10	C11	H11B	109.5
H11A	C11	H11B	109.5	C10	C11	H11C	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5
C10	C12	H12A	109.5	C10	C12	H12B	109.5
H12A	C12	H12B	109.5	C10	C12	H12C	109.5
H12A	C12	H12C	109.5	H12B	C12	H12C	109.5
C10	C13	H13A	109.5	C10	C13	H13B	109.5
H13A	C13	H13B	109.5	C10	C13	H13C	109.5
H13A	C13	H13C	109.5	H13B	C13	H13C	109.5
C17	C14	C16	105.4(6)	C17	C14	C4	111.4(6)
C16	C14	C4	110.9(6)	C17	C14	C15	108.9(6)
C16	C14	C15	108.0(6)	C4	C14	C15	112.0(6)
C14	C15	H15A	109.5	C14	C15	H15B	109.5
H15A	C15	H15B	109.5	C14	C15	H15C	109.5
H15A	C15	H15C	109.5	H15B	C15	H15C	109.5
C14	C16	H16A	109.5	C14	C16	H16B	109.5
H16A	C16	H16B	109.5	C14	C16	H16C	109.5
H16A	C16	H16C	109.5	H16B	C16	H16C	109.5
C14	C17	H17A	109.5	C14	C17	H17B	109.5
H17A	C17	H17B	109.5	C14	C17	H17C	109.5
H17A	C17	H17C	109.5	H17B	C17	H17C	109.5
C22	C18	C19	106.8(6)	C22	C18	C23	126.8(6)
C19	C18	C23	126.3(7)	C22	C18	Ce1	77.0(5)
C19	C18	Ce1	78.6(4)	C23	C18	Ce1	108.4(4)

C18	C19	C20	109.1(7)	C18	C19	Ce1	72.3(4)
C20	C19	Ce1	81.1(4)	C18	C19	H19	125.5
C20	C19	H19	125.5	Ce1	C19	H19	113.3
C21	C20	C19	106.6(6)	C21	C20	C27	133.1(6)
C19	C20	C27	118.8(6)	C21	C20	Ce1	76.2(4)
C19	C20	Ce1	70.2(4)	C27	C20	Ce1	128.6(5)
C22	C21	C20	106.6(6)	C22	C21	C31	118.2(6)
C20	C21	C31	133.0(6)	C22	C21	Ce1	68.7(4)
C20	C21	Ce1	76.1(4)	C31	C21	Ce1	132.0(5)
C18	C22	C21	110.9(6)	C18	C22	Ce1	73.8(4)
C21	C22	Ce1	83.1(4)	C18	C22	H22	124.6
C21	C22	H22	124.6	Ce1	C22	H22	110.6
C18	C23	C26	111.7(6)	C18	C23	C24	110.1(6)
C26	C23	C24	107.1(6)	C18	C23	C25	109.8(6)
C26	C23	C25	110.1(6)	C24	C23	C25	108.1(6)
C23	C24	H24A	109.5	C23	C24	H24B	109.5
H24A	C24	H24B	109.5	C23	C24	H24C	109.5
H24A	C24	H24C	109.5	H24B	C24	H24C	109.5
C23	C25	H25A	109.5	C23	C25	H25B	109.5
H25A	C25	H25B	109.5	C23	C25	H25C	109.5
H25A	C25	H25C	109.5	H25B	C25	H25C	109.5
C23	C26	H26A	109.5	C23	C26	H26B	109.5
H26A	C26	H26B	109.5	C23	C26	H26C	109.5
H26A	C26	H26C	109.5	H26B	C26	H26C	109.5
C28	C27	C30	107.2(6)	C28	C27	C20	111.7(6)
C30	C27	C20	110.7(6)	C28	C27	C29	106.3(6)
C30	C27	C29	109.7(6)	C20	C27	C29	111.1(6)
C27	C28	H28A	109.5	C27	C28	H28B	109.5
H28A	C28	H28B	109.5	C27	C28	H28C	109.5
H28A	C28	H28C	109.5	H28B	C28	H28C	109.5
C27	C29	H29A	109.5	C27	C29	H29B	109.5
H29A	C29	H29B	109.5	C27	C29	H29C	109.5
H29A	C29	H29C	109.5	H29B	C29	H29C	109.5
C27	C30	H30A	109.5	C27	C30	H30B	109.5
H30A	C30	H30B	109.5	C27	C30	H30C	109.5
H30A	C30	H30C	109.5	H30B	C30	H30C	109.5
C34	C31	C32	108.6(6)	C34	C31	C33	105.4(6)
C32	C31	C33	105.6(6)	C34	C31	C21	108.5(6)
C32	C31	C21	117.9(6)	C33	C31	C21	110.0(5)
C31	C32	H32A	109.5	C31	C32	H32B	109.5
H32A	C32	H32B	109.5	C31	C32	H32C	109.5
H32A	C32	H32C	109.5	H32B	C32	H32C	109.5
C31	C33	H33A	109.5	C31	C33	H33B	109.5
H33A	C33	H33B	109.5	C31	C33	H33C	109.5
H33A	C33	H33C	109.5	H33B	C33	H33C	109.5
C31	C34	H34A	109.5	C31	C34	H34B	109.5

H34A	C34	H34B	109.5	C31	C34	H34C	109.5
H34A	C34	H34C	109.5	H34B	C34	H34C	109.5
C36	C35	Ce1	91.7(4)	C36	C35	H35A	113.3
Ce1	C35	H35A	113.3	C36	C35	H35B	113.3
Ce1	C35	H35B	113.3	H35A	C35	H35B	110.7
C41	C36	C35	123.6(8)	C41	C36	C37	110.8(7)
C35	C36	C37	125.4(7)	C41	C36	Ce1	87.8(4)
C35	C36	Ce1	60.1(4)	C37	C36	Ce1	122.3(5)
C38	C37	C36	123.1(7)	C38	C37	H37	118.5
C36	C37	H37	118.5	C37	C38	C39	120.4(8)
C37	C38	H38	119.8	C39	C38	H38	119.8
C38	C39	C40	117.1(7)	C38	C39	C42	119.5(8)
C40	C39	C42	123.4(7)	C41	C40	C39	119.1(7)
C41	C40	H40	120.4	C39	C40	H40	120.4
C40	C41	C36	129.4(8)	C40	C41	H41	115.3
C36	C41	H41	115.3	C39	C42	H42A	109.5
C39	C42	H42B	109.5	H42A	C42	H42B	109.5
C39	C42	H42C	109.5	H42A	C42	H42C	109.5
H42B	C42	H42C	109.5	C44	C43	H10A	109.5
C44	C43	H10B	109.5	H10A	C43	H10B	109.5
C44	C43	H10C	109.5	H10A	C43	H10C	109.5
H10B	C43	H10C	109.5	C45	C44	C43	144(2)
C45	C44	H10D	101.0	C43	C44	H10D	101.0
C45	C44	H10E	101.0	C43	C44	H10E	101.0
H10D	C44	H10E	104.5	C46	C45	C44	131.3(13)
C46	C45	H10F	104.4	C44	C45	H10F	104.4
C46	C45	H10G	104.4	C44	C45	H10G	104.4
H10F	C45	H10G	105.6	C47	C46	C45	150(3)
C47	C46	H10H	99.1	C45	C46	H10H	99.1
C47	C46	H10I	99.1	C45	C46	H10I	99.1
H10H	C46	H10I	104.0	C46	C47	H10J	109.5
C46	C47	H10K	109.5	H10J	C47	H10K	109.5
C46	C47	H10L	109.5	H10J	C47	H10L	109.5
H10K	C47	H10L	109.5	C35	Ce1	C18	111.6(2)
C35	Ce1	C2	128.6(2)	C18	Ce1	C2	118.5(2)
C35	Ce1	C22	130.7(2)	C18	Ce1	C22	29.2(2)
C2	Ce1	C22	93.0(2)	C35	Ce1	C1	99.7(2)
C18	Ce1	C1	145.0(2)	C2	Ce1	C1	29.11(18)
C22	Ce1	C1	116.4(2)	C35	Ce1	C19	85.3(2)
C18	Ce1	C19	29.07(19)	C2	Ce1	C19	138.9(2)
C22	Ce1	C19	47.1(2)	C1	Ce1	C19	151.3(2)
C35	Ce1	C5	87.0(2)	C18	Ce1	C5	158.88(19)
C2	Ce1	C5	46.9(2)	C22	Ce1	C5	139.7(2)
C1	Ce1	C5	29.13(19)	C19	Ce1	C5	171.9(2)
C35	Ce1	C3	131.5(2)	C18	Ce1	C3	113.0(2)
C2	Ce1	C3	28.46(17)	C22	Ce1	C3	97.8(2)

C1	Ce1	C3	47.61(18)	C19	Ce1	C3	141.7(2)
C5	Ce1	C3	46.32(19)	C35	Ce1	C20	86.3(2)
C18	Ce1	C20	47.69(18)	C2	Ce1	C20	119.6(2)
C22	Ce1	C20	46.46(19)	C1	Ce1	C20	122.77(19)
C19	Ce1	C20	28.77(19)	C5	Ce1	C20	148.26(19)
C3	Ce1	C20	139.17(19)	C35	Ce1	C21	112.3(2)
C18	Ce1	C21	47.5(2)	C2	Ce1	C21	94.3(2)
C22	Ce1	C21	28.20(17)	C1	Ce1	C21	106.6(2)
C19	Ce1	C21	46.7(2)	C5	Ce1	C21	135.7(2)
C3	Ce1	C21	111.41(19)	C20	Ce1	C21	27.77(18)
C35	Ce1	C36	28.20(19)	C18	Ce1	C36	95.9(2)
C2	Ce1	C36	143.5(2)	C22	Ce1	C36	123.2(2)
C1	Ce1	C36	119.0(2)	C19	Ce1	C36	77.5(2)
C5	Ce1	C36	96.6(2)	C3	Ce1	C36	128.5(2)
C20	Ce1	C36	91.9(2)	C21	Ce1	C36	119.4(2)
C35	Ce1	C4	104.7(2)	C18	Ce1	C4	132.05(19)
C2	Ce1	C4	46.16(19)	C22	Ce1	C4	124.4(2)
C1	Ce1	C4	47.09(18)	C19	Ce1	C4	158.43(19)
C5	Ce1	C4	27.82(17)	C3	Ce1	C4	27.65(18)
C20	Ce1	C4	165.62(19)	C21	Ce1	C4	138.39(19)
C36	Ce1	C4	102.2(2)				

2.5 Least-squares planes for $Cp'_2Ce[4\text{-methylbenzyl}] \bullet 0.5(pentane)$

Plane number 1

Atoms defining plane	Distance
C(1)	0.023(5)
C(2)	-0.016(5)
C(3)	0.003(4)
C(4)	0.011(5)
C(5)	-0.021(5)

Plane number 2

Atoms defining plane	Distance
C(18)	0.009(5)
C(19)	-0.001(5)
C(20)	-0.006(5)
C(21)	0.012(4)
C(22)	-0.013(5)

Plane number 3

Atoms defining plane	Distance
Ce(1)	0
C(35)	0
C(36)	0

Plane number 4

Atoms defining plane	Distance
C(36)	-0.011(5)
C(37)	0.011(5)
C(38)	-0.007(5)
C(39)	0.003(5)
C(40)	-0.003(5)
C(41)	0.008(5)

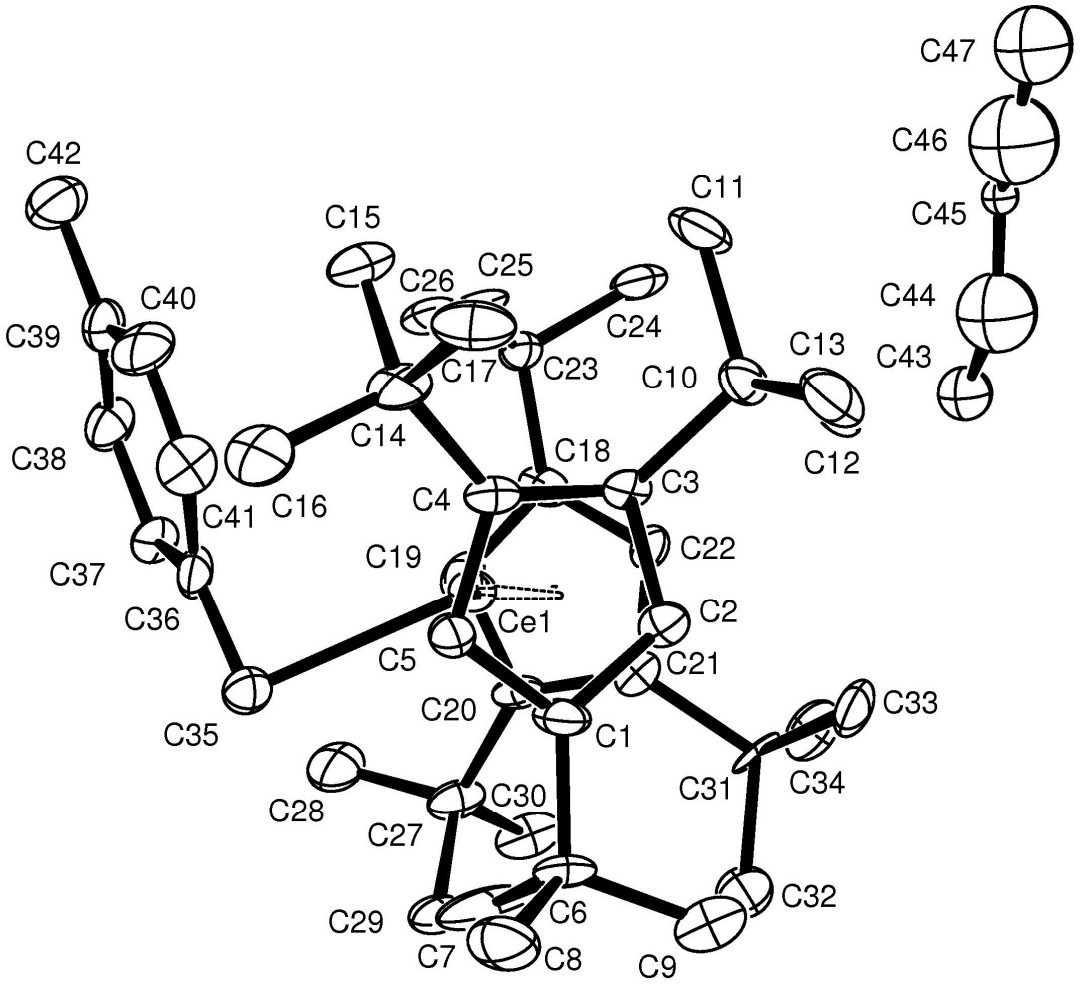
Summary

plane	RMS deviation
1	0.0164
2	0.0091
3	0.0000
4	0.0081

Dihedral angles between planes (°)

plane	1	2	3
2	43.20		
3		20.56	
4			66.79

2.6 ORTEP (50% ellipsoids) showing atom labeling scheme for $Cp'_2Ce[4\text{-methylbenzyl}] \bullet 0.5(pentane)$



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(3) Least-Squares:

Function minimized $\Sigma w(|F_o|-|F_c|)^2$

where $w = 4F_o^2/2(F_o^2) = [\sigma^2(F_o) + (pF_o/2)^2]^{-1}$

$F_o^2 = S(C-RB)/Lp$

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

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(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

(10) SMART: Area-Detector Software Package, Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(11) SAINT: SAX Area-Dectector Integration Program, V4.024; Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(12) SADABS: Bruker-Nonius Area Detector Scaling and Absorption v. 2.05 Bruker Analytical X-ray Systems, Inc.: Madison, WI (2003).

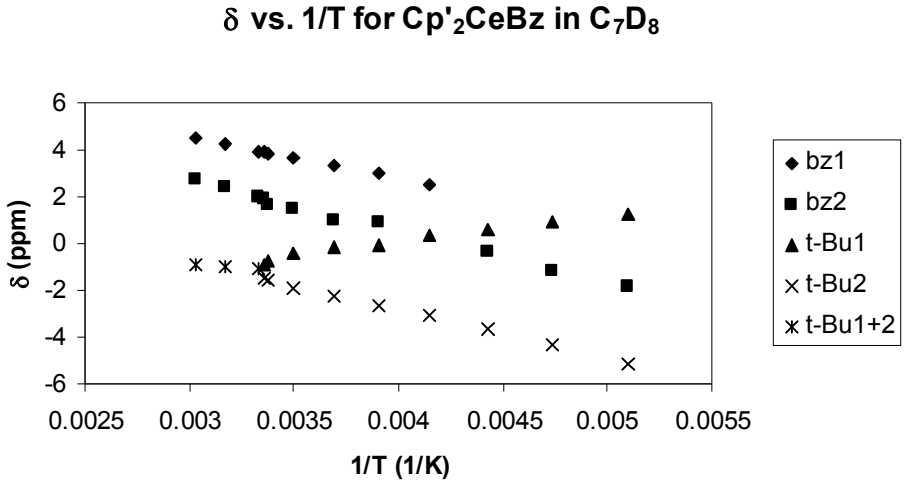
(13)XPREP:(v 6.12) Part of the SHELXTL Crystal Structure Determination Package, Bruker AXS Inc.: Madison, WI, (1995)

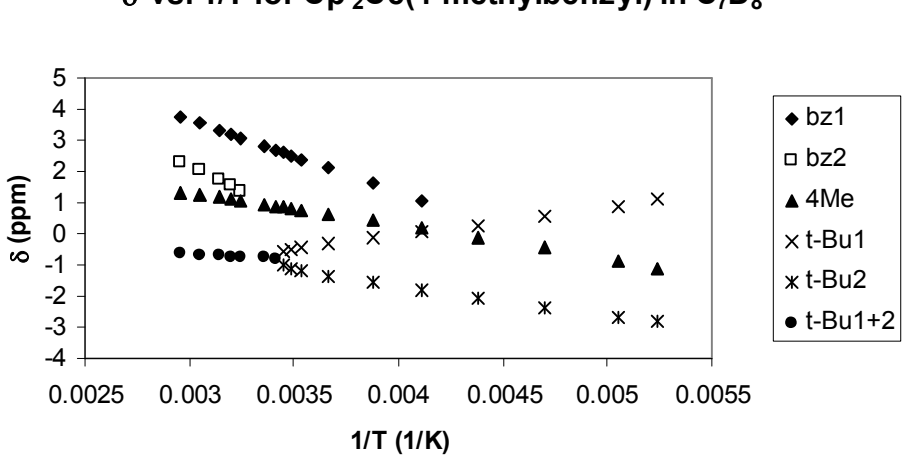
(14) XS: Program for the Solution of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(15) XL: Program for the Refinement of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(16) XP: Molecular Graphics program. Part of the SHELXTL Structure Determination Package. Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

4. δ vs. 1/T plots





5 Coordinates (x, y, z), E and G (a.u.) for all stationary points.

Cp2CeCH2Ph

35
E=-690.1556916 G=-689.921397

C	.363258	-.532326	3.134789
C	1.227605	-1.075557	2.147892
C	1.811673	.003431	1.439083
C	1.300220	1.210888	1.978826
C	.412755	.878423	3.031415
Ce	-.871733	.018011	.629510
C	-1.269416	.773907	-2.072527
C	.132809	.631913	-1.915005
C	.418321	-.746750	-1.743536
C	-.808525	-1.454258	-1.778701
C	-1.851158	-.513997	-1.985778
C	-2.423307	2.103041	1.084401
H	2.544673	-.078089	.645851
H	1.574316	2.213549	1.671135
H	-.115914	1.584165	3.660680
H	-.199103	-1.098699	3.868647
H	1.445826	-2.127475	1.999065
H	1.402924	-1.185463	-1.634621
H	-.924475	-2.530991	-1.713842
H	-2.903385	-.746407	-2.091978
H	-1.797055	1.701870	-2.254089
H	.863303	1.431265	-1.966826
H	-2.668040	2.760469	.251969
C	-3.350587	1.037528	1.355263
H	-2.025088	2.630244	1.951505
C	-4.257710	.546807	.369576
C	-5.002701	-.608609	.563564
C	-4.868826	-1.371600	1.730849
C	-3.976585	-.937605	2.707647
C	-3.223609	.227434	2.525861
H	-4.389838	1.124457	-.542049
H	-5.702828	-.922035	-.207319
H	-5.455982	-2.273180	1.874320
H	-3.868081	-1.497681	3.633585
H	-2.582267	.575824	3.333015

CH3F

5
E=-64.2072796 G=-64.190228

C	0.791982	-0.054326	0.034892
H	0.285789	-0.130731	1.001655
H	1.876369	-0.054297	0.179137
H	0.499855	-0.890060	-0.607687
F	0.420814	1.129415	-0.573053

Adduct complex Cp2CeCH2Ph and CH3F

```
40
E=-754.3719188 G=-754.103963
 C        -.626267   -2.556276   -1.786025
 C       -1.812851   -1.838403   -1.492812
 C       -1.555536    -.462356   -1.714646
 C        -.211332    -.326872   -2.138827
 C         .363272   -1.623596   -2.184304
Ce         .015279   -1.144375     .558765
 C        1.372009     .655217    2.313866
 C        2.039905    -.573293    2.510962
 C        2.744748    -.885887    1.317625
 C        2.518221     .160287     .390453
 C        1.658196    1.107691     .999359
 C       -1.462049   -2.410337    2.387671
 C       -3.010074     .784315    1.730746
 F       -1.682050     .766688    1.276112
 H       -3.104035     .026833    2.508716
 H       -3.657225     .556862     .881904
 H       -3.206320    1.785723    2.117342
 H        2.942097     .231925    -.604275
 H        1.316963    2.036901     .557303
 H         .760356    1.171990    3.044295
 H        2.045519   -1.153389    3.426669
 H        3.388292   -1.744515    1.162698
 H         .280039     .599013   -2.414426
 H        1.371638   -1.862207   -2.503266
 H        -.501236   -3.630121   -1.715502
 H       -2.755583   -2.274074   -1.184167
 H       -2.268882     .347640   -1.611341
 C        -.946165   -3.597028    1.758009
 H        -.934703   -2.089258    3.290984
 H       -2.545515   -2.370348    2.500546
 C         .459608   -3.829545    1.674777
 C         .990669   -4.903817     .941748
 C         .158135   -5.773255     .254282
 C       -1.231447   -5.562349     .315287
 C       -1.766491   -4.504808    1.025778
 H        1.127611   -3.249380    2.312320
 H        2.066943   -5.060620     .938756
 H         .566024   -6.608534    -.306478
 H       -1.900131   -6.245880    -.203211
 H       -2.845155   -4.369618    1.062023
```

TS sigma bond metathesis

```
40
E=-754.294935 G=-754.030941
 C    -0.441649     0.598270    -2.693864
 C     0.638636     1.319953    -2.124233
 C     1.680432     0.399296    -1.841664
 C     1.236589    -0.890698    -2.217616
 C    -0.075565    -0.766033    -2.747542
Ce    -0.357443    -0.199964     0.034739
 C    -0.310350    -0.184997     2.885524
 C     0.784224    -1.008308     2.517870
 C     1.767598    -0.187060     1.913070
 C     1.278735     1.144099     1.902285
```

C	-0.004190	1.143671	2.508018
F	-2.565029	0.338078	0.064638
C	-3.519083	-1.513523	0.005806
C	-1.177251	-2.747539	0.074303
H	2.738199	-0.512033	1.556050
H	1.811804	2.015153	1.538499
H	-0.632579	2.011954	2.672288
H	-1.211865	-0.510072	3.391946
H	0.870955	-2.072728	2.704086
H	2.654468	0.645601	-1.435826
H	1.816306	-1.805497	-2.161581
H	-0.674647	-1.572698	-3.153767
H	-1.379343	1.021787	-3.034617
H	0.683202	2.394206	-1.981944
H	-3.342461	-2.318270	0.702267
H	-4.227069	-0.752091	0.295227
H	-3.426680	-1.731416	-1.048920
H	-1.454721	-3.144597	1.052915
H	-1.712373	-3.245113	-0.734444
C	-0.109373	-3.713453	-0.096420
C	0.567956	-4.213171	1.022288
C	1.599011	-5.145778	0.857452
C	1.952736	-5.578667	-0.426092
C	1.275407	-5.078949	-1.544800
C	0.244353	-4.146342	-1.379964
H	0.292808	-3.876445	2.020702
H	2.125876	-5.534487	1.727647
H	2.754750	-6.304102	-0.554311
H	1.550555	-5.415675	-2.543214
H	-0.282513	-3.757633	-2.250159

Transition state Proton transfer

40
E=-754.3270668 G=-754.059989

C	-.515697	-2.518772	-1.790064
C	-1.756000	-1.850233	-1.635563
C	-1.549427	-.475070	-1.905413
C	-.180301	-.288523	-2.213650
C	.459304	-1.555255	-2.145327
Ce	-.151786	-.934626	.514518
C	1.198019	.828408	2.279479
C	1.790838	-.427621	2.549282
C	2.537810	-.814898	1.406738
C	2.410753	.208293	.434627
C	1.577756	1.221155	.971750
C	-1.470719	-2.347582	2.610191
C	-2.378083	.213518	1.619596
F	-1.686194	1.169842	.776167
H	-1.842293	-1.079824	2.024143
H	-3.352381	.051062	1.146949
H	-2.520409	.718218	2.580377
H	2.889964	.226451	-.536898
H	1.295844	2.144440	.479295
H	.577991	1.401544	2.958604
H	1.720176	-.976066	3.481601
H	3.140873	-1.710466	1.309322

H	.287670	.649082	-2.490330
H	1.501250	-1.755685	-2.367333
H	-.347337	-3.581303	-1.663603
H	-2.701812	-2.318634	-1.390055
H	-2.303970	.301905	-1.882489
C	-1.002747	-3.509628	1.830576
H	-.803673	-2.107719	3.444986
H	-2.479883	-2.505383	3.003938
C	.378288	-3.781819	1.672652
C	.828850	-4.847020	.885608
C	-.077947	-5.674370	.231623
C	-1.447871	-5.422334	.374135
C	-1.900881	-4.360543	1.144807
H	1.100362	-3.202143	2.245799
H	1.896258	-5.038283	.809151
H	.269006	-6.509673	-.368985
H	-2.169230	-6.068395	-.120024
H	-2.969489	-4.189690	1.253028

Adduct of Cp2CeCH2F and toluene

40
E=-754.3606298 G=-754.105139

C	-.256149	-2.016269	-2.155905
C	-1.552266	-2.065329	-1.578910
C	-2.071175	-.749969	-1.551971
C	-1.095857	.116745	-2.108868
C	.020983	-.668188	-2.491195
Ce	.032682	-.692834	.337248
C	2.018667	1.212721	.932067
C	1.897401	.482263	2.140551
C	2.422448	-.813509	1.920049
C	2.867669	-.887190	.574566
C	2.622202	.369186	-.033404
C	-2.564917	-3.310604	3.043516
C	-1.713212	.137107	1.995012
F	-1.299855	1.252804	1.085362
H	-2.432732	-2.232435	3.167012
H	-2.797670	.081880	1.847432
H	-1.521857	.541736	2.995083
H	3.363682	-1.731279	.108154
H	2.880721	.645618	-1.048753
H	1.718893	2.243267	.781010
H	1.496419	.859364	3.073559
H	2.519563	-1.593380	2.667748
H	-1.202569	1.186502	-2.248174
H	.917827	-.304039	-2.978603
H	.387787	-2.866590	-2.348591
H	-2.060041	-2.958816	-1.235714
H	-3.045598	-.454266	-1.181995
C	-1.576341	-3.859147	2.051596
H	-2.429536	-3.779109	4.025858
H	-3.594668	-3.497821	2.727735
C	-.245085	-3.406289	2.041203
C	.693619	-3.950849	1.158948
C	.315549	-4.953431	.262670
C	-.999955	-5.409522	.264829

```
 C       -1.933437   -4.865313    1.148564
 H         .066678   -2.661132    2.773443
 H        1.724897   -3.609643    1.191444
 H        1.044974   -5.380821    -.418909
 H       -1.304463   -6.193137    -.423536
 H       -2.956691   -5.233104    1.141919
```

Transition state for insertion of CH2 into Toluene

```
40
E=-754.3178831 G=-754.053889
 C        .743354    -.045369    2.749415
 C        .646658    1.321583    2.384014
 C       1.669632    1.601124    1.444661
 C       2.394826     .404580    1.223218
 C       1.824245    -.610436    2.035321
Ce       -.121052    -.153768     .020551
 C        .681625    -.738866   -2.634336
 C       -.709210    -.514016   -2.759686
 C       -.946432     .867006   -2.558354
 C        .301540    1.499085   -2.315359
 C       1.307786     .506162   -2.361831
 F      -1.045667   -2.094405     .371813
 C      -2.458734    1.083996     .639610
 C      -2.132041    3.374505     .188566
 H      -3.372391     .810257     .079341
 H      -2.782435    1.307334    1.666670
 H       1.888371    2.566327    1.001579
 H       3.265132     .296434     .586183
 H       2.165401   -1.636939    2.109015
 H        .111769    -.565437    3.460183
 H       -.050464    2.039174    2.802984
 H      -1.910159    1.358332   -2.637135
 H        .471045    2.561639   -2.176852
 H       2.372716     .673927   -2.252062
 H       1.183929   -1.692086   -2.757218
 H      -1.458105   -1.268036   -2.970563
 C      -3.233671    4.352882     .320687
 H      -1.626306    3.356231    -.777441
 H      -1.418514    3.350410    1.008290
 H      -2.652892    2.298343     .142363
 C      -3.585602    4.861679    1.579687
 C      -4.616488    5.787483    1.699458
 C      -5.310981    6.208297     .564558
 C      -4.971498    5.704602    -.691935
 C      -3.940408    4.779661    -.813988
 H      -3.042171    4.534895    2.462751
 H      -4.877607    6.183263    2.676335
 H      -6.116006    6.931358     .658933
 H      -5.509200    6.035408   -1.575436
 H      -3.672738    4.389291   -1.792849
```

Transition state IA

```
40
E:  -754.331268  G:  -754.058656
Ce    -0.834491     0.132883     0.517756
```

C	0.408146	0.214860	3.085410
C	0.118448	-1.155048	2.851984
C	0.945726	-1.603567	1.792683
C	1.743306	-0.509880	1.367709
C	1.414342	0.608864	2.171877
C	-1.790718	-1.597493	-1.511283
C	-0.416358	-1.902165	-1.351116
C	0.336243	-0.801735	-1.839583
C	-0.575985	0.176314	-2.306791
C	-1.887993	-0.311317	-2.102049
H	-0.310357	1.132562	-2.740922
H	-2.804729	0.194594	-2.379050
H	-2.616391	-2.256097	-1.268568
H	-0.011838	-2.832451	-0.972013
H	1.416330	-0.736921	-1.886659
H	1.854451	1.595754	2.093831
H	2.501562	-0.535677	0.594930
H	0.994067	-2.615104	1.408757
H	-0.575278	-1.767609	3.416126
H	-0.039490	0.840410	3.847949
C	-3.548363	3.678507	1.366214
H	-3.313287	4.313338	2.215842
H	-4.050856	4.158510	0.530936
C	-3.626537	2.301901	1.531552
C	-3.079250	1.628214	2.684520
C	-3.022476	0.248219	2.783629
C	-3.428279	-0.589639	1.719922
C	-3.986937	0.038690	0.584148
C	-4.047965	1.417083	0.472347
H	-2.755025	2.233499	3.528838
H	-2.644400	-0.197968	3.699868
H	-3.460161	-1.668647	1.836666
H	-4.367686	-0.572368	-0.230207
H	-4.486951	1.857032	-0.421245
C	-1.311905	3.231017	0.421784
F	0.009950	2.406644	-0.077858
H	-2.045000	2.766047	-0.224456
H	-1.034310	4.251164	0.180762
H	-1.286888	2.960463	1.469548

Adduct between Cp2CeF and ethylbenzene

40
E=-754.4572535 G=-754.189043

C	-0.972122	1.563600	2.248081
C	0.410196	1.825078	2.029931
C	1.080879	0.584184	1.926991
C	0.114214	-0.446813	2.057019
C	-1.151123	0.163591	2.272757
Ce	-0.518060	0.715982	-0.412127
C	1.399261	-0.854202	-1.726158
C	0.342766	-0.736038	-2.669808
C	0.309546	0.599955	-3.124160
C	1.352466	1.312480	-2.470157
C	2.032867	0.410384	-1.618500
F	-2.576074	0.281344	-0.958309
C	-1.501026	3.758562	-1.594844

C	-2.573882	4.744478	-1.117031
H	-1.959384	2.788007	-1.825728
H	-0.722866	3.649588	-0.822890
H	2.146589	0.442711	1.792909
H	0.318542	-1.511972	2.066170
H	-2.090981	-0.354050	2.424533
H	-1.748414	2.306268	2.393366
H	0.877360	2.804148	2.012898
H	-0.375173	1.001689	-3.862075
H	1.621578	2.349043	-2.642718
H	2.898080	0.638939	-1.007515
H	1.711962	-1.766179	-1.230005
H	-0.320705	-1.531352	-2.989336
C	-3.255279	4.318593	0.162825
H	-3.320148	4.855280	-1.913932
H	-2.120486	5.732182	-0.978767
H	-1.005318	4.107624	-2.505652
C	-3.118152	5.072649	1.333442
C	-3.745636	4.681285	2.516361
C	-4.521341	3.523403	2.545202
C	-4.662489	2.760839	1.385471
C	-4.035353	3.154697	0.205165
H	-2.519091	5.980824	1.316891
H	-3.629397	5.283090	3.413704
H	-5.012489	3.217125	3.464607
H	-5.261155	1.854429	1.395388
H	-4.151529	2.541213	-0.684791

Cp2CeF

22

E= -443.680124591 / G = -443.555131 au

C	0.731608	1.144301	-2.242715
C	1.505363	0.018316	-1.864449
C	0.738534	-1.144339	-2.119384
C	-0.502835	-0.735796	-2.683506
C	-0.505600	0.673610	-2.762154
Ce	-0.634278	0.116493	0.001444
C	0.747110	-1.142122	2.117705
C	1.511694	0.021359	1.859779
C	0.737971	1.146529	2.240551
C	-0.496841	0.674517	2.764431
C	-0.492735	-0.734888	2.686080
H	2.519001	0.046530	1.461633
H	1.062508	2.181305	2.208941
H	-1.298100	1.285651	3.163433
H	-1.286417	-1.390941	3.025904
H	1.078373	-2.165200	1.976135
H	2.514144	0.042400	-1.469996
H	1.069134	-2.167764	-1.978767
H	-1.298383	-1.391047	-3.020501
H	-1.307458	1.285569	-3.158692
H	1.057482	2.178698	-2.212543
F	-2.777407	0.396910	0.006939

CH3CH2Ph

18

E=-310.7722787 G=-310.647093

C	1.227686	0.000641	-0.755256
C	0.013364	0.231489	-0.110647
C	-0.044123	0.265768	1.281419
C	1.105427	0.070825	2.055755
C	2.317782	-0.158289	1.394675
C	2.381315	-0.193953	0.003051
H	-0.890809	0.390124	-0.692631
H	-0.994833	0.451706	1.777132
C	1.033774	0.069072	3.564149
H	3.223744	-0.305455	1.979316
H	3.334032	-0.368992	-0.489994
H	1.275534	-0.022786	-1.840500
H	1.971649	0.462741	3.974538
H	0.241186	0.751896	3.893301
C	0.773510	-1.326362	4.145046
H	0.728487	-1.295412	5.238805
H	-0.173989	-1.733751	3.777751
H	1.565964	-2.024940	3.857713