Electronic Supporting Information for

Fast and reversible insertion of carbon dioxide into zirconcene-alkoxide bonds. A mechanistic study

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Contents

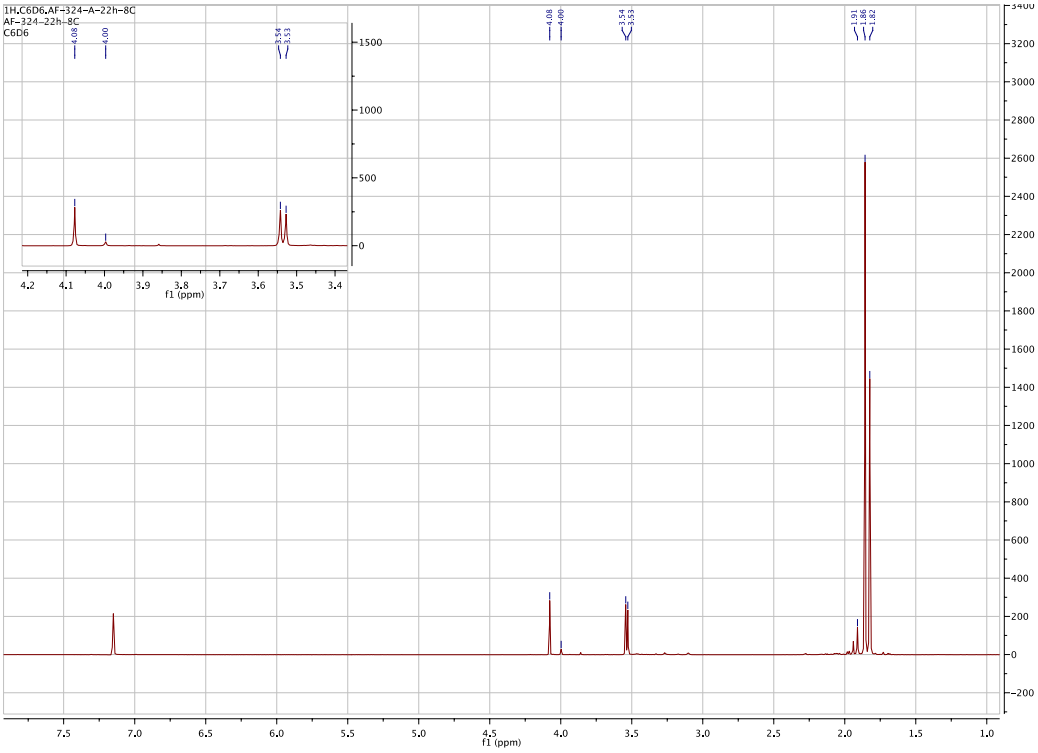
1. NMR-spectra.....S2

2. Thermodynamic and kinetic data and figures.....S5

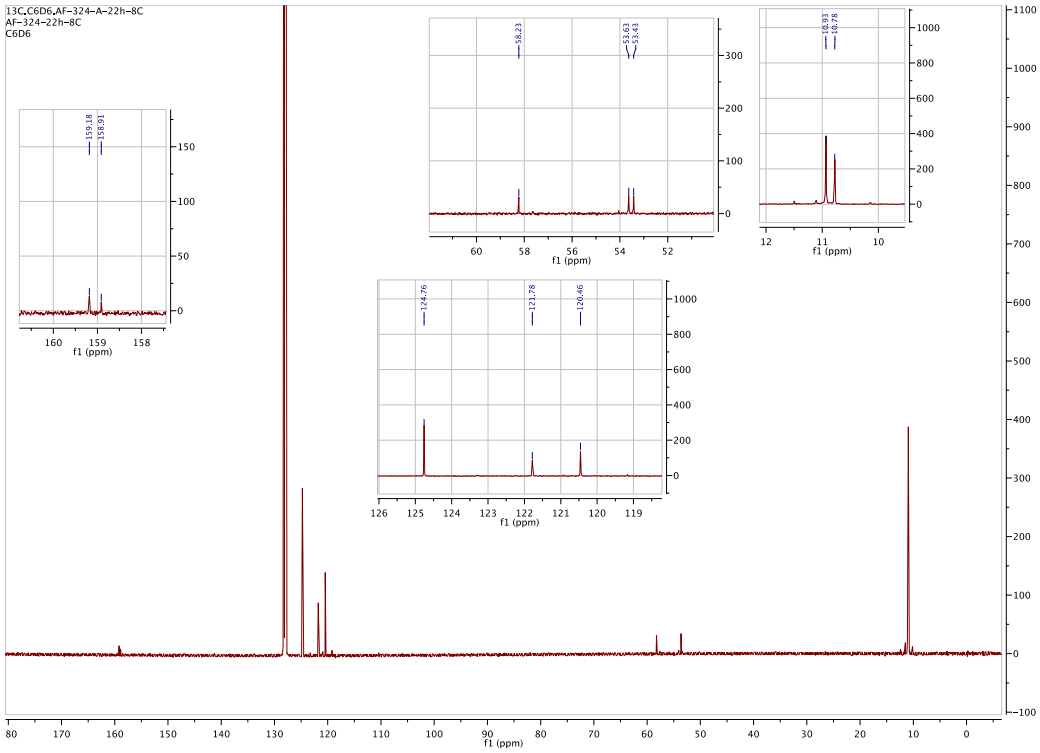
3. Computational details S8

1. NMR-spectra

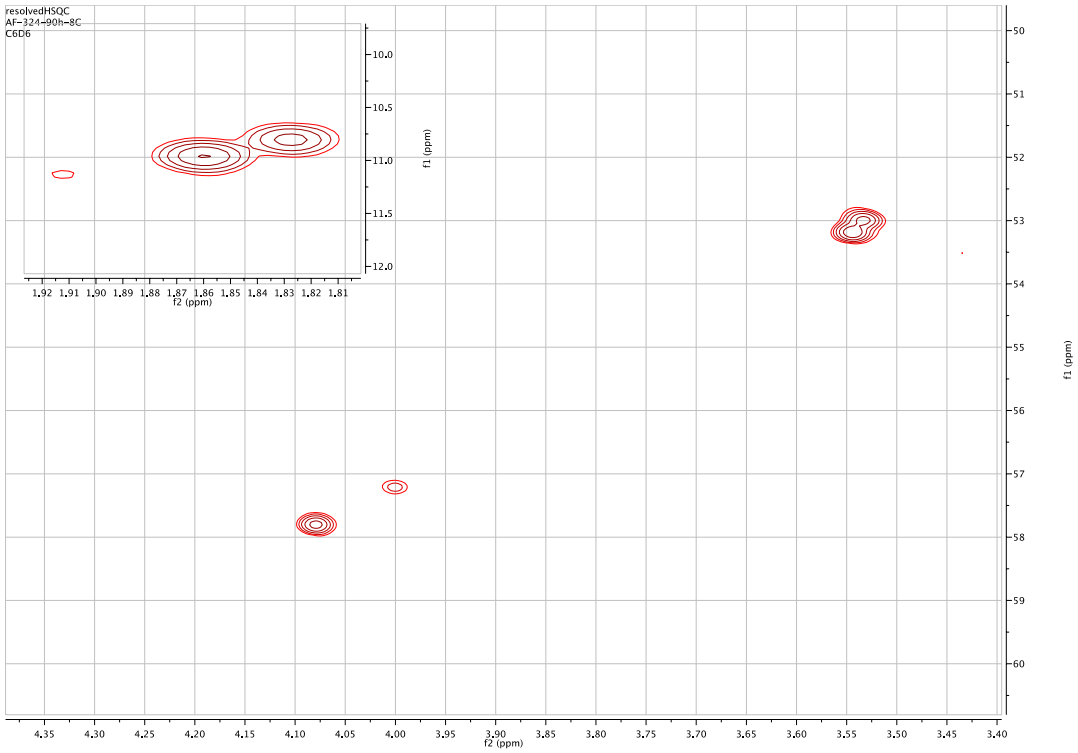
^{1}H-NMR (C_6D_6) of the equilibrium mixture. To maximise products, all spectra were recorded at the highest carbon dioxide pressure at 8 °C. The composition in the spectra is 5% **1**, 60% **3** and 35% **4**.



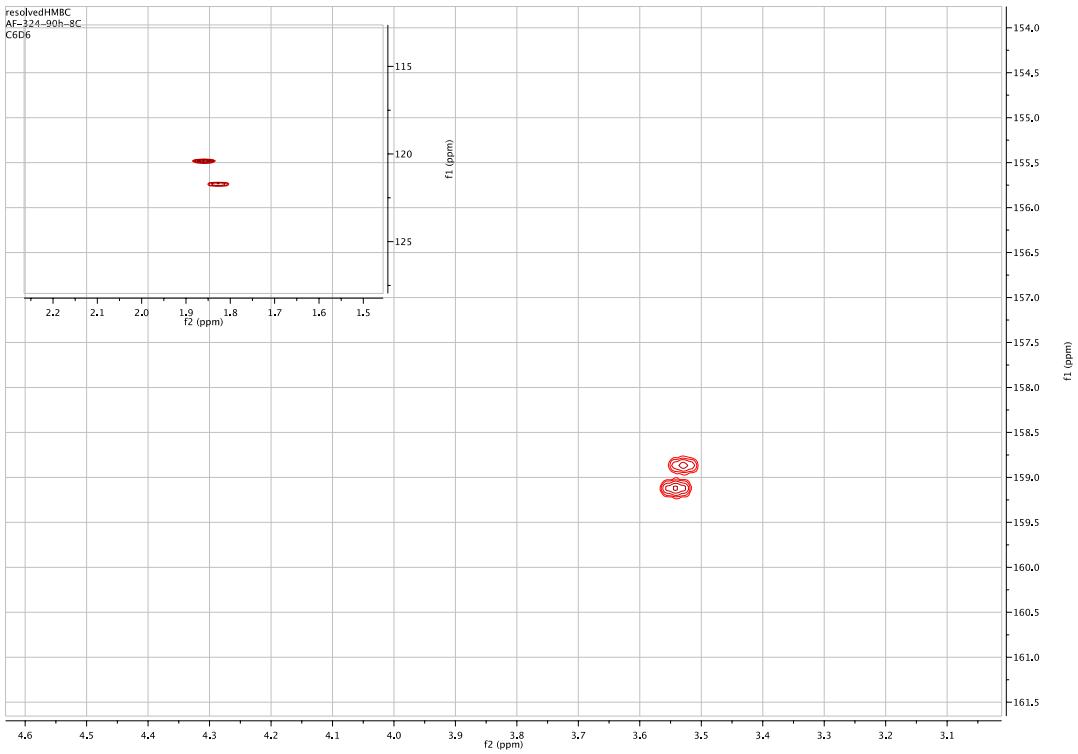
^{13}C-NMR (C_6D_6) of the equilibrium mixture. The peak at 124.8 ppm is CO_2. Due to its low concentration only trace peaks of **1** are visible.



^{1}H {^{13}C} HSQC spectrum of the equilibrium mixture



^{1}H {^{13}C} HMBC spectrum of the equilibrium mixture



2. Thermodynamic and kinetic data and figures

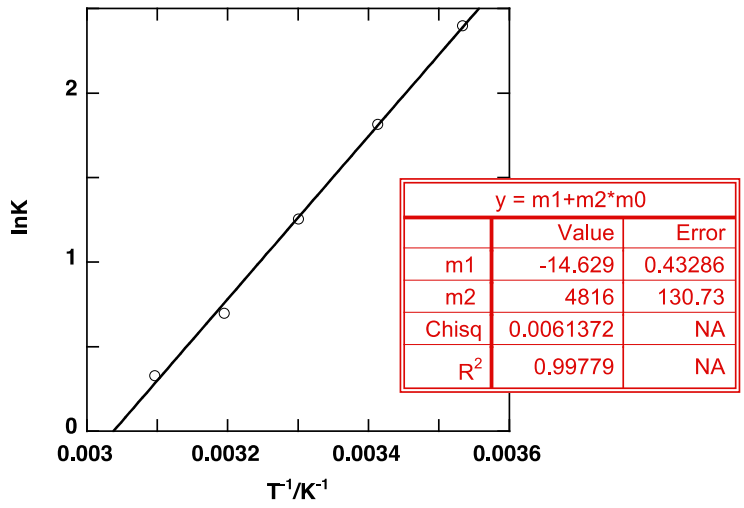


Figure S1. A van´t Hoff plot for equilibrium K_1. Equilibrium constants were determined at different temperatures from the slopes in Figure 1.

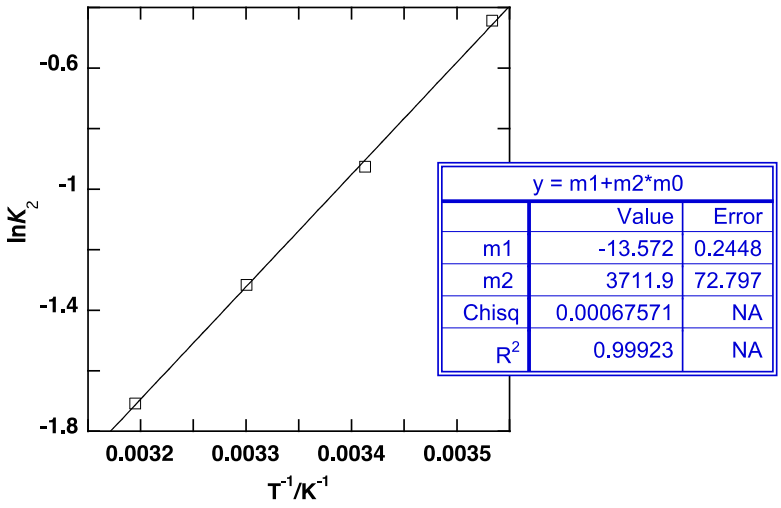


Figure S2. A van´t Hoff plot for equilibrium K_2. Equilibrium constants were determined from the ratio of [**4**]/[**3**] at 283-313 K and a loading of 6.3 atm CO_2 (at 298 K prior to equilibration).

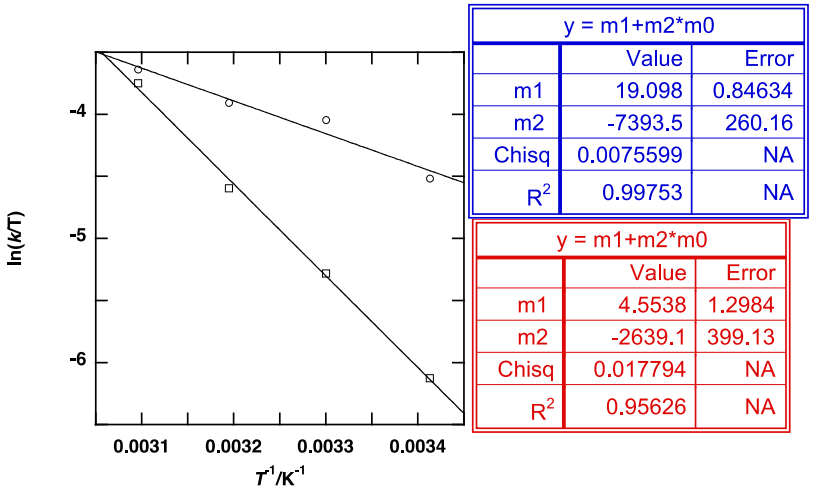


Figure S3. Eyring plot for the forward and reverse reactions of the first equilibrium.

Table S1. Kinetic data obtained from the magnetisation transfer evaluation of the first equilibrium in Scheme 2. [Zr] = 13 mM.

Entry	T/K	[CO_2]/M	k_{obs}/s^{-1}	k_{-1}/s^{-1}	$1/T_1^1$/s^{-1}	$1/T_1^4$/s^{-1}
1	293	0.114	0.590±0.006	0.70	0.29	0.30
2	293	0.230	0.971±0.022	0.63	0.54	0.24
3	293	0.366	1.385±0.034	0.58	0.59	0.40
4	303	0.102	0.717±0.019	1.60	0.22	0.29
5	303	0.211	1.421±0.024	1.56	0.34	0.25
6	303	0.340	1.88±0.04	1.46	0.49	0.17
7	313	0.0900	0.73±0.34	2.66	0.33	0.18
8	313	0.192	1.74±0.07	3.49	0.34	0.16
9	313	0.313	2.42±0.15	3.34	0.42	0.20
10	323	0.0778	1.21±0.14	8.52	0.23	0.18
11	323	0.173	2.12±0.11	7.48	0.28	0.18
12	323	0.286	2.94±0.21	6.80	0.33	0.21

Table S2. Kinetic and thermodynamic data

T/K	k_1/M^{-1}s^{-1}	k_{-1}/s^{-1}	K_1[a]/M^{-1}	K_1[b]/M^{-1}	K_2[c]/M^{-1}
283			11.02±0.14		0.642
293	3.20±0.12	0.64±0.07	6.15±0.06	5.0±0.6	0.396
303	5.31±0.18	1.54±0.08	3.5±0.4	3.4±0.1	0.268
313	6.3±1.3	3.2±0.5	2.01±0.09	2.0±0.5	0.181
323	8.5±1.2	7.6±0.9	1.39±0.05	1.1±0.2	

[a] From the slope of Figure 1. [b] From the k_1/k_{-1} ratio. [c] The error is <5%.

3. Computational details

All geometries were optimized at the B3LYP-D3/LACVP* level. Frequencies and thermodynamic corrections were calculated at the same level. Single point energies in solvent were calculated at the final geometries using the PBF method with parameters for benzene: dielectric constant 2.284, probe molecule radius 2.600 Å.

Cartesian coordinates and energies for all complexes:

$Cp^*_2Zr(OMe)_2$

```
File: Zr_Cpstar2_OMe2_f.out; structure: final
Method: DFT(b3lyp-d3)/lacvp*
SCF energy: -1057.28739380561 au
Gibbs free energy: -1056.816081 au
Low frequencies 22.58 39.31 66.04 82.16 86.80 94.20
Solution phase energy: -1057.28920024628 au
Zr1          -0.0624161859     -0.1939758211      0.0344097862
C2           -0.1053148402      0.5519836273      2.5148351282
C3            1.2780056632      0.3920395038      2.1911752133
C4            1.5274893592     -0.9945484815      1.9909549500
C5            0.2824386798     -1.6897741993      2.1422133952
C6           -0.7122756333     -0.7309602107      2.4956532727
C7            1.8991974887     -0.8170073658     -1.5817119479
C8            1.1250460784      0.1427300936     -2.2967102839
C9           -0.1536637631     -0.4233424390     -2.5575469227
C10          -0.1601922985     -1.7520952275     -2.0299844691
C11           1.1090013300     -2.0060420924     -1.4441718830
C12           0.0784500825     -3.1821213935      2.1517285807
H13          -0.7678035233     -3.4890800739      1.5232174336
H14           0.9633921133     -3.7124390709      1.7921487090
H15          -0.1309813647     -3.5444755047      3.1674288680
C16          -2.1384040715     -1.0479131528      2.8395800331
H17          -2.4822701990     -1.9500657831      2.3243548798
H18          -2.2527030705     -1.2183150894      3.9189858823
H19          -2.8096548048     -0.2330184441      2.5556635568
C20          -0.7606338026      1.8604858438      2.8471120913
H21          -0.5189393983      2.1761977814      3.8712943119
H22          -0.4209485325      2.6405887831      2.1594507582
H23          -1.8506071778      1.7964817554      2.7671494715
C24           2.2704792798      1.5192319616      2.1259641962
H25           3.2293442533      1.1932858433      1.7100464368
H26           1.8840193222      2.3256247510      1.4923538845
H27           2.4680078878      1.9379005478      3.1220215318
C28           2.8892749242     -1.6306141592      1.9526488731
H29           2.8994769641     -2.5771280668      1.4079518935
H30           3.6370326301     -0.9755248780      1.5009184410
H31           3.2247674130     -1.8467649457      2.9770117824
C32           1.6405887228      1.4929814114     -2.7039236770
H33           0.9933311689      1.9661750522     -3.4481276604
H34           1.7035919144      2.1657755380     -1.8404909515
H35           2.6424490307      1.4076709332     -3.1424364006
```

C36	-1.3013769801	0.2233568333	-3.2862697691
H37	-1.7216628488	-0.4546847593	-4.0386711877
H38	-2.1099493444	0.5010342455	-2.6008992579
H39	-0.9835169713	1.1330614403	-3.8039485465
C40	-1.2733567214	-2.7560336147	-2.1578496932
H41	-1.4659146468	-3.2763574992	-1.2115649581
H42	-2.2076486811	-2.2777067339	-2.4613322695
H43	-1.0323318304	-3.5239935741	-2.9061150669
C44	1.5824105227	-3.3731207757	-1.0361937335
H45	0.8024809649	-3.9407309752	-0.5196181592
H46	1.8659078949	-3.9533421010	-1.9260141445
H47	2.4578070652	-3.3347097083	-0.3852669012
C48	3.3643175420	-0.6518673503	-1.2795285953
H49	3.7673045873	-1.5115489780	-0.7405140616
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H51	3.5652375539	0.2446847007	-0.6807840474
O54	-2.0295758840	-0.3663295456	-0.1141515178
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H58	-3.6720323206	-0.6803915735	-1.3253069658
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C60	-0.8935986799	2.6719955691	-0.7813594604
H61	-0.8077484961	3.6928335307	-0.3805033048
H62	-0.6942052800	2.7167523615	-1.8626227800
H63	-1.9346130862	2.3361417460	-0.6489171558

CO_2

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Low frequencies 643.65 643.65 1370.11 2435.17
Total Quantum Mechanical Energy: -188.581859599

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$Cp^*_2Zr(OMe)$-$O(Me)\cdots CO_2$, TS

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Solution phase energy: -1245.86918045828 au

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C3	1.2580178625	0.1139598934	2.2674443805
C4	1.6444523111	-1.0787280885	1.5987847544
C5	0.5038638169	-1.9518810339	1.5806627628
C6	-0.5731129816	-1.2832871829	2.2332242068
C7	1.2634222562	-0.4822203017	-2.2025339477
C8	0.3395990211	0.5623558923	-2.5134107560

C9	-0.9754599903	0.0287629366	-2.4242594189
C10	-0.8761653582	-1.3381319582	-2.0301789156
C11	0.5130289757	-1.6602746259	-1.9189888771
C12	0.4835659328	-3.4258496854	1.2825832729
H13	-0.3974257980	-3.7223437362	0.7029882546
H14	1.3718981854	-3.7525297671	0.7411982780
H15	0.4496022740	-3.9906613260	2.2249904196
C16	-1.9097083135	-1.9164130857	2.4987646415
H17	-2.3918504152	-2.2461200128	1.5714475116
H18	-1.7964135330	-2.7986779494	3.1430299917
H19	-2.5950447198	-1.2273596700	2.9976605849
C20	-0.8399719045	1.0405006604	3.4425621685
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H22	-0.9042398446	1.9917642132	2.9020892942
H23	-1.8537958445	0.7268814973	3.7037028068
C24	2.1348816567	1.2586651963	2.6844171772
H25	3.0975146530	1.2474921499	2.1709927020
H26	1.6549864601	2.2232986394	2.4847341480
H27	2.3233469618	1.2093091632	3.7660924477
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H43	-2.4421124301	-2.6025845262	-2.8228540159
C44	1.1021931564	-3.0429591017	-1.8914483709
H45	0.4174783651	-3.7824349151	-1.4724507495
H46	1.3316808287	-3.3578223128	-2.9193907233
H47	2.0395377546	-3.0889373525	-1.3302437865
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H49	3.2698909216	-1.1061218039	-1.6898089809
H50	3.0177437421	-0.7680293607	-3.4045180354
H51	3.1566416997	0.5615105717	-2.2378306275
O52	2.3177005678	1.5726769514	-0.2329530683
C53	1.8069821226	2.6582654548	-0.1093344462
O54	1.8664578027	3.8430649952	-0.0844834785
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C56	-0.9777362014	3.1233691884	0.1630552116
H57	-0.5137173114	4.1161999041	0.1813128689
H58	-1.5821607630	3.0243649646	-0.7481130409
H59	-1.6433158398	3.0222496760	1.0290732088
O60	-2.0782640308	0.1989097482	0.1798378369
C61	-3.2385364340	0.5682487408	0.8580425715
H62	-3.0351068867	0.9517567361	1.8664676285
H63	-3.7647855900	1.3558502908	0.2974441023
H64	-3.9206168953	-0.2894532370	0.9529349486

$Cp^*_2Zr(OMe)$-OCOOMe

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Gibbs free energy: -1245.402798 au
Low frequencies 19.35 25.53 46.23 58.86 79.57 88.97
Solution phase energy: -1245.89233148104 au

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C3	1.0926223577	0.3739277992	2.3351882046
C4	1.3290975240	-0.9964507047	2.0607200502
C5	0.0531807814	-1.6527000444	1.9818703540
C6	-0.9571373888	-0.6773397080	2.2456599894
C7	1.9102856468	-0.9963928026	-1.6607443232
C8	1.1750457679	-0.0299335567	-2.4162186323
C9	-0.1542296034	-0.5072712683	-2.5767274649
C10	-0.2574077751	-1.7631268864	-1.9113675999
C11	1.0312417098	-2.0855070476	-1.3737061638
C12	-0.2096313751	-3.1345805919	1.9680973983
H13	-0.9843178330	-3.4151029553	1.2458515793
H14	0.6902962808	-3.7065426277	1.7374145202
H15	-0.5608435734	-3.4623258416	2.9564757126
C16	-2.4241834249	-0.9903936973	2.3405012145
H17	-2.8637145155	-1.1700427780	1.3525800472
H18	-2.5868600412	-1.8871148198	2.9506897754
H19	-2.9778278671	-0.1701535683	2.8058612351
C20	-0.9519903360	1.9022861987	2.7644305189
H21	-0.6046876779	2.2650774365	3.7400800214
H22	-0.6864037300	2.6603061123	2.0179979057
H23	-2.0419635310	1.8373192230	2.8012908115
C24	2.1397770492	1.4085245846	2.6343771487
H25	3.0333071907	1.2815131500	2.0198604817
H26	1.7603113208	2.4187920170	2.4554586537
H27	2.4367957535	1.3508579772	3.6909570836
C28	2.6902746641	-1.6350850646	2.0838257934
H29	2.6858200077	-2.6371816018	1.6499756995
H30	3.4283597877	-1.0362493861	1.5412456838
H31	3.0479416064	-1.7298600878	3.1186064600
C32	1.7318335881	1.2109281975	-3.0548361367
H33	1.0748389334	2.0733109626	-2.8968653679
H34	2.7116467795	1.4631109199	-2.6473962275
H35	1.8323934583	1.0669992062	-4.1388126458
C36	-1.2589268513	0.1625586692	-3.3386625642
H37	-2.2021932058	0.0920179838	-2.7892276613
H38	-1.0464757650	1.2238329905	-3.5006832783
H39	-1.3965284709	-0.3067452642	-4.3223677243
C40	-1.5005785420	-2.6081597293	-1.8666015328
H41	-1.4278802201	-3.4013609234	-1.1156911894
H42	-2.3714509648	-1.9911915268	-1.6197786692
H43	-1.6941299996	-3.0893753581	-2.8347797658
C44	1.4612017568	-3.4547515103	-0.9244576829
H45	0.6313745549	-4.0382114999	-0.5210705895
H46	1.8582672901	-4.0098461822	-1.7860411517
H47	2.2529056644	-3.4256786284	-0.1726805067
C48	3.3886570381	-0.9332546242	-1.3816553523
H49	3.7042694670	-1.7382208493	-0.7124953814
H50	3.9629412211	-1.0378402020	-2.3124339574
H51	3.6623643647	0.0239084750	-0.9269912530
O52	0.7241448015	1.9412953488	-0.1740173988

C53	1.8235944152	2.6327042473	-0.2547450554
O54	2.9707346921	2.2019299451	-0.2991877363
O55	1.5464628047	3.9647570435	-0.2791969870
C56	2.6954711825	4.8132800689	-0.3817691480
H57	2.3074929879	5.8337822178	-0.3853098907
H58	3.3697201024	4.6641541912	0.4674552857
H59	3.2477714337	4.6129854076	-1.3054083621
O60	-1.8064265802	0.3788921068	-0.4264085287
C61	-2.6851633424	1.4213659142	-0.0925658597
H62	-3.4329469598	1.5432089938	-0.8894162764
H63	-3.2196243590	1.2157143393	0.8454842480
H64	-2.1462839793	2.3732662217	0.0217323154

Cp*$_2$Zr(OCOOMe)-O(Me)···CO$_2$, TS

File: Zr_Cpstar2_OCOOMe_OMe_CO2_c_f_tsf.out; structure: final
Method: DFT(b3lyp-d3)/lacvp*
SCF energy: -1434.46495294082 au
Gibbs free energy: -1433.969990 au
Low frequencies -209.61 24.72 36.27 49.85 57.94 60.87
Solution phase energy: -1434.47073354434 au

Zr1	0.1690029286	0.0415299853	0.1416332269
C2	-0.0150669583	-0.1826804288	2.7108093736
C3	1.3767417906	-0.1031383429	2.4389391064
C4	1.7547682317	-1.2636337187	1.6930836003
C5	0.5896476146	-2.0928074034	1.5660339417
C6	-0.4998495405	-1.4160750170	2.1768338501
C7	1.4455559981	-0.3779012962	-2.1083540937
C8	0.5162991302	0.6830737147	-2.3372351219
C9	-0.7967055862	0.1480525457	-2.2288731666
C10	-0.6896763514	-1.2463844685	-1.9184293082
C11	0.6991939545	-1.5705015876	-1.8744629377
C12	0.5350521615	-3.5413527038	1.1693511671
H13	-0.3385555107	-3.7692866945	0.5505662963
H14	1.4286850947	-3.8632849523	0.6339706095
H15	0.4546606978	-4.1610150723	2.0734567618
C16	-1.8869473534	-1.9752325247	2.3322413620
H17	-2.3282157111	-2.2694881168	1.3749977066
H18	-1.8718507870	-2.8610110448	2.9818366144
H19	-2.5606367147	-1.2441950975	2.7864459140
C20	-0.8222366290	0.8284566007	3.4745523077
H21	-0.9418635221	0.5258135142	4.5238263923
H22	-0.3341966801	1.8075842113	3.4669366240
H23	-1.8177775723	0.9553558001	3.0411547188
C24	2.2878002119	0.9748847374	2.9529835196
H25	3.2795646133	0.9187185965	2.5002644180
H26	1.8824734533	1.9735734932	2.7562770243
H27	2.4061286981	0.8802225733	4.0402749097
C28	3.1622073916	-1.6298068169	1.3086786270
H29	3.1803644111	-2.4104339355	0.5428640987
H30	3.7051788989	-0.7653652004	0.9160228249
H31	3.7199850442	-2.0101697207	2.1751317343
C32	0.8421445706	2.0966595675	-2.7273164703
H33	0.2734190260	2.8193385565	-2.1355496566
H34	1.9032021059	2.3196200038	-2.5884754062
H35	0.6026319041	2.2700414168	-3.7845129507
C36	-2.0631638662	0.9101907029	-2.4990497428
H37	-2.9389659708	0.3771242816	-2.1256266233

H38	-2.0470358728	1.8997527865	-2.0294970303
H39	-2.1909372268	1.0619236204	-3.5795939391
C40	-1.8366857689	-2.2161534697	-1.8209404085
H41	-1.5391297842	-3.1368299808	-1.3084499897
H42	-2.6809845640	-1.7855341378	-1.2758697785
H43	-2.1878219978	-2.5022495012	-2.8221127692
C44	1.3036192253	-2.9447170587	-1.9358363162
H45	0.6178413563	-3.7200873204	-1.5922276182
H46	1.5605148865	-3.1757172978	-2.9794762076
H47	2.2296714325	-3.0219333576	-1.3589911390
C48	2.9329857385	-0.3480898382	-2.3244590470
H49	3.4700633692	-0.8980987479	-1.5455888703
H50	3.1804432806	-0.8149398997	-3.2882792303
H51	3.3253412883	0.6696448970	-2.3304397659
O52	2.6697203409	1.3423512640	0.0105024420
C53	2.3138354902	2.4736119441	0.2007846632
O54	2.4628817505	3.6366178620	0.3312832086
O55	0.4137184508	2.1134136869	0.4240652656
C56	-0.5102957285	3.1679713212	0.6036959696
H57	0.0417291702	4.0646412469	0.9104623952
H58	-1.0444798844	3.3890352997	-0.3313267638
H59	-1.2519369397	2.9028618656	1.3631166461
O60	-1.8355742599	0.4301128643	0.4533250524
C61	-3.1270227039	0.4073832734	0.5376378144
O62	-3.8909495055	-0.4193743687	0.0586179470
O63	-3.5723628278	1.4703771719	1.2716675274
C64	-4.9960482953	1.5472550444	1.4179178160
H65	-5.1806540962	2.4397432824	2.0188937347
H66	-5.3847432790	0.6582376554	1.9242068644
H67	-5.4839263654	1.6363193715	0.4423727004

$Cp^*_2Zr(OCOOMe)_2$

File: Zr_Cpstar2_OCOOMe2_f2.out; structure: final
Method: DFT(b3lyp-d3)/lacvp*
SCF energy: -1434.48500820464 au
Gibbs free energy: -1433.988512 au
Low frequencies 17.78 23.85 31.72 46.81 50.97 69.62
Solution phase energy: -1434.49254138078 au

Zr1	0.2455967155	0.1490204577	-0.0414134596
C2	0.0984262037	0.8967182031	2.3967555434
C3	1.3759591438	0.2742078391	2.2531137958
C4	1.1724653072	-1.1114164707	2.0031195018
C5	-0.2440562691	-1.3534428603	1.9917142542
C6	-0.8954960432	-0.1161347302	2.2657850923
C7	1.8588418111	-0.8900350548	-1.7420096129
C8	1.0655884370	0.0595427959	-2.4633908452
C9	-0.2757047961	-0.4100963150	-2.4877894708
C10	-0.3283855537	-1.6484275753	-1.7740691165
C11	1.0010268713	-1.9635283445	-1.3524268949
C12	-0.9452505745	-2.6840474049	1.9473318638
H13	-1.8416815774	-2.6499490465	1.3196661185
H14	-0.2983252042	-3.4763849977	1.5642255048
H15	-1.2644888829	-2.9820343272	2.9554754405
C16	-2.3696500458	0.0584879447	2.4885876001
H17	-2.9604797831	-0.6164005654	1.8649165042
H18	-2.6149917630	-0.1471966049	3.5392765988
H19	-2.6897615234	1.0808480515	2.2699133521

C20	-0.1540665674	2.3563396645	2.6528634865
H21	-0.1595993496	2.5750411084	3.7290077151
H22	0.6073516523	2.9794191167	2.1767249953
H23	-1.1197077225	2.6628189738	2.2400557097
C24	2.7200764394	0.9233591101	2.4314242372
H25	3.4068850557	0.6866784155	1.6130510502
H26	2.6325078411	2.0114884476	2.4807932315
H27	3.1859509827	0.5843798190	3.3667511023
C28	2.2782519253	-2.1279461441	2.0612458339
H29	1.9329840148	-3.1303518347	1.8067934850
H30	3.1103740562	-1.8722366576	1.3976782785
H31	2.6846767637	-2.1690016136	3.0810846783
C32	1.5667031580	1.2966336678	-3.1533929429
H33	0.8619166481	2.1277189235	-3.0440876319
H34	2.5278704351	1.6180296287	-2.7480001652
H35	1.6920380448	1.1078555365	-4.2283538360
C36	-1.4158661879	0.2454470846	-3.2136104635
H37	-2.3762026985	-0.1524388029	-2.8804610032
H38	-1.4261976658	1.3279720047	-3.0487604515
H39	-1.3278105778	0.0735691143	-4.2947592162
C40	-1.5299454373	-2.5488496158	-1.6676072297
H41	-1.3507850195	-3.3668284535	-0.9648309698
H42	-2.4110970880	-1.9944929057	-1.3338908741
H43	-1.7592571732	-2.9992658374	-2.6429076972
C44	1.4505923815	-3.3244475198	-0.9003451810
H45	0.7666112579	-3.7796841732	-0.1811585808
H46	1.4908983031	-3.9936925818	-1.7709188837
H47	2.4485153474	-3.3047689115	-0.4607396199
C48	3.3537568244	-0.8304124795	-1.5777989450
H49	3.7027575854	-1.5309383420	-0.8127271357
H50	3.8549468923	-1.1002764868	-2.5174697295
H51	3.6819293759	0.1732001513	-1.2942787818
O52	1.3093482220	1.9120764435	-0.1934164250
C53	2.3903477653	2.6338798029	-0.2078687393
O54	3.5116388427	2.2832922324	-0.5509953320
O55	2.1243257513	3.8930559519	0.2334989419
C56	3.2486213341	4.7821771950	0.2305325255
H57	2.8673861347	5.7362126703	0.5990366446
H58	4.0427897663	4.4086292857	0.8844694168
H59	3.6517426790	4.8967303492	-0.7802334777
O60	-1.5935651758	1.0717025782	-0.3110201822
C61	-2.8808593817	0.9102453365	-0.4135935888
O62	-3.4825942963	-0.1418710410	-0.5952089877
O63	-3.5190082863	2.1009795972	-0.2771644766
C64	-4.9467836638	2.0318350771	-0.3728409354
H65	-5.2980730966	3.0577826155	-0.2485103485
H66	-5.2548702983	1.6377899904	-1.3461495343
H67	-5.3587954415	1.3893828496	0.4118417901