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Reversible Metal-free Carbon Dioxide Binding by Frustrated Lewis Pairs**

Cornelia M. Mömming[a], Edwin Otten[b], Gerald Kehr[a], Roland Fröhlich[a], Stefan Grimme[a], Douglas W. Stephan[b] and Gerhard Erker*[a]*

General Procedures. All syntheses involving air- and moisture-sensitive compounds were carried out using standard Schlenk-type glassware (or in a glove box) under an atmosphere of argon. Solvents were dried with the procedure according to Grubbs (A. B. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen, F. J. Timmers, *Organometallics* **1996**, *15*, 1518-1520) or were distilled from appropriate drying agents and stored under an argon atmosphere. NMR spectra were recorded on a *Varian* Inova 500 (^{1}H: 499.9 MHz, ^{13}C: 125.7 MHz, ^{19}F: 470.3 MHz, ^{11}B: 160.4 MHz, ^{31}P: 202.3 MHz). ^{1}H NMR and ^{13}C NMR: chemical shift d is given relative to TMS and referenced to the solvent signal. ^{19}F NMR: chemical shift d is given relative to $CFCl_3$ (external reference); ^{11}B NMR: chemical shift d is given relative to $BF_3{\cdot}Et_2O$ (external reference); ^{31}P NMR: chemical shift d is given relative to H_3PO_4 (85% in D_2O) (external reference). NMR assignments are supported by additional 2D NMR experiments. Elemental analyses were performed on a *Elementar Vario El III*. IR spectra were recorded on a *Varian* 3100 FT-IR (Excalibur Series). Melting points were obtained with a DSC Q20 (*TA Instruments*).

X Ray Crystal Structure Analyses. Data sets were collected with a Nonius KappaCCD diffractometer. Programs used: data collection COLLECT (Nonius B.V., 1998), data reduction Denzo-SMN (Z. Otwinowski, W. Minor, *Methods in Enzymology*, **1997**, *276*, 307-326), absorption correction Denzo (Z. Otwinowski, D. Borek, W. Majewski, W. Minor, *Acta Cryst.* **2003**, *A59*, 228-234), structure solution SHELXS-97 (G.M. Sheldrick, *Acta Cryst.* **1990**, *A46*, 467-473), structure refinement SHELXL-97 (G.M. Sheldrick, Universität Göttingen, 1997), graphics XP (BrukerAXS, 2000).

[*] [a]Cornelia M. Mömming, Dr. Gerald Kehr, Dr. Roland Fröhlich, Professor Dr. Stefan Grimme, Professor Dr. Gerhard Erker
Organisch-Chemisches Institut der Universität Münster, Corrensstrasse 40, 48149 Münster, Germany
E-mail: erker@uni-muenster.de

[b]Dr. Edwin Otten, Professor Dr. Douglas W. Stephan
Department of Chemistry, University of Toronto, 80 St. George St. Toronto Ontario Canada, M5S 3H6
E-mail: dstephan@chem.utoronto.ca
Homepage: http://www.chem.utoronto.ca/staff/DSTEPHAN

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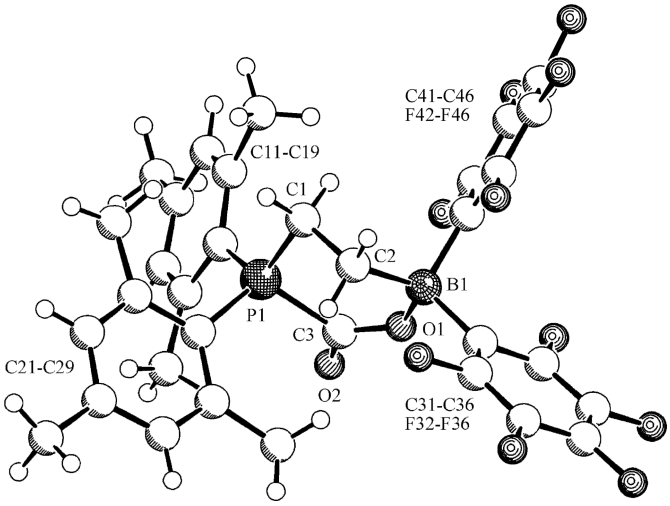
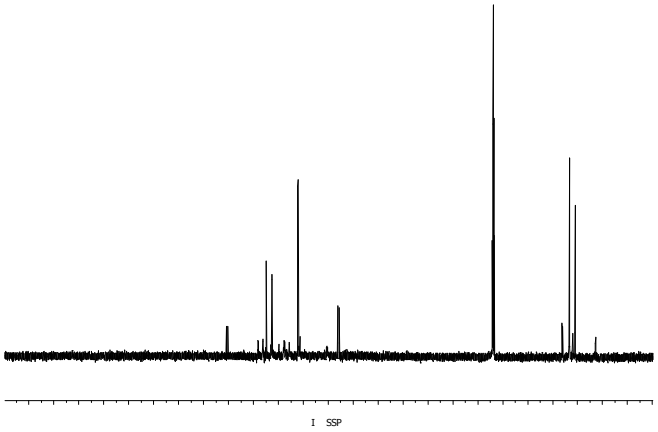
Materials. Dimesitylvinylphosphine (P. Spies, G. Erker, G. Kehr, K. Bergander, R. Fröhlich, S. Grimme, D. W. Stephan, *Chem. Commun*. **2007**, *47*, 5072-5074) and $HB(C_6F_5)_2$ (a) D. J. Parks, R. E. von H. Spence, W. E. Piers, *Angew. Chem.* **1995**, *107*, 895-897; Angew. Chem. *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 809-811; b) W. E. Piers, D. J. Parks, G. P. A. Yap, *Organometallics* **1998**, *17*, 5492-5503) were prepared according to literature procedures. Carbon dioxide (5.0) was used without further purification.

Synthesis of (3). Dimesitylvinylphosphine (100 mg, 0.34 mmol) and $HB(C_6F_5)_2$ (117 mg, 0.34 mmol) were dissolved in pentane (7 mL) and stirred for 15 min. After degassing the solution, carbon dioxide (2 bar) was introduced for 30 minutes whereupon a white powder precipitated after 5 minutes. The precipitate was collected via cannula filtration after 2 hours and washed twice with pentane (2 mL). All volatiles were removed in vacuo to yield **3** (184 mg, 79%). Anal. Calc. for $C_{33}H_{26}BF_{10}O_2P$: C, 57.75; H, 3.82. Found C, 57.49; H, 3.68. Crystals suitable for X-Ray analysis were grown from a layered dichloromethane/ pentane solution under a CO_2 pressure of 2 bar at –36 °C .^{1}H NMR (500 MHz, 223 K, $[D_2]CH_2Cl_2$) d = 7.00 (4H, d, $^2J_{PH}$ = 4.3 Hz, *m*-Mes), 3.06 (2H, m, ^{P}CH$_2$), 2.30 (6H, s, *p*-CH_3^{Mes}), 2.21 (12 H, s, *o*-CH_3^{Mes}), 1.47 (2H, dm, $^3J_{PH}$ = 28.8 Hz, ^{B}CH$_2$). ^{13}C{^{1}H} NMR (126 MHz, 223 K, $[D_2]CH_2Cl_2$) d = 160.5 (d, $^1J_{PC}$ = 89.0 Hz, C=O), 147.2 (dm, $^1J_{FC}$ = 237 Hz, C_6F_5), 144.9 (d, $^4J_{PC}$ = 2.1 Hz, *p*-Mes), 142.6 (d, $^2J_{PC}$ = 9.2 Hz, *o*-Mes), 138.9 (dm, $^1J_{FC}$ = 254 Hz, C_6F_5), 136.6 (dm, $^1J_{FC}$ = 254 Hz, C_6F_5), 132.1 (d, $^3J_{PC}$ = 11.4 Hz, *m*-Mes), 120.5 (br, *i*-C_6F_5), 115.9 (d, $^1J_{PC}$ = 73.6 Hz, *i*-Mes), 26.1 (d, $^1J_{PC}$ = 34.4 Hz, ^{P}CH$_2$), 23.2 (d, $^3J_{PC}$ = 4.2 Hz, *o*-CH_3^{Mes}), 20.9 (*p*-CH_3^{Mes}), 12.7 (br, ^{B}CH$_2$). ^{1}H TOCSY (500 MHz, 223 K, $[D_2]CH_2Cl_2$) d $^1H_{irr}$ / d $^1H_{res}$ = 7.00 / 2.30, 2.21 (*m*-Mes / *p*-CH_3^{Mes}, *o*-CH_3^{Mes}), 3.06 / 1.47 (^{P}CH$_2$ / ^{B}CH$_2$); APT (125 MHz, 223 K, $[D_2]CH_2Cl_2$) d = 160.5 (up, C=O), 147.2 (up, C_6F_5), 144.9 (up, *p*-Mes), 142.7 (up, *o*-Mes), 138.9 (up, C_6F_5), 136.6 (up, C_6F_5), 132.1 (down, *m*-Mes), 120.3 (up *i*-C_6F_5), 115.9 (up, *i*-Mes), 26.1 (up, ^{P}CH$_2$), 23.2 (down, *o*-CH_3^{Mes}), 20.9 (down, *p*-CH_3^{Mes}), 12.7 (up, ^{B}CH$_2$); ^{1}H,^{13}C GHSQC (500 MHz / 125 MHz, 223 K, $[D_2]CH_2Cl_2$) d (^{1}H) / d (^{13}C) = 7.00 / 132.1 (*m*-Mes), 3.06 / 26.1 (^{P}CH$_2$), 2.30 / 20.9 (*p*-CH_3^{Mes}), 2.21 / 23.2 (*o*-CH_3^{Mes}); ^{1}H,^{13}C GHMBC (500 MHz / 125 MHz, 223 K, $[D_2]CH_2Cl_2$) d (^{1}H) / d (^{13}C) = 7.00 / 142.7, 132.1, 115.9, 23.2, 20.9 (*m*-Mes / *o*-Mes, *m*-Mes, *i*-Mes, *o*-CH_3^{Mes}, *p*-CH_3^{Mes}), 3.06 / 160.5, 115.9, 12.7 (^{P}CH$_2$ / C=O, *i*-Mes, ^{B}CH$_2$), 2.30 / 144.9, 132.1 (*p*-CH_3^{Mes} / *p*-Mes, *m*-Mes), 2.21 / 142.6, 132.1, 115.9 (*o*-CH_3^{Mes} / *o*-Mes, *m*-Mes, *i*-Mes), 1.47 / 26.1 (^{B}CH$_2$ / ^{P}CH$_2$), ^{11}B{^{1}H} NMR (160 MHz, 223 K, $[D_2]CH_2Cl_2$) d = –2.4. ^{31}P{^{1}H} NMR (202 MHz, 223 K, $[D_2]CH_2Cl_2$) d = 0.6 (?$_{1/2}$ = 6 Hz). ^{19}F NMR (470 MHz, 223 K, $[D_2]CH_2Cl_2$) d = –135.6 (4F, *o*-

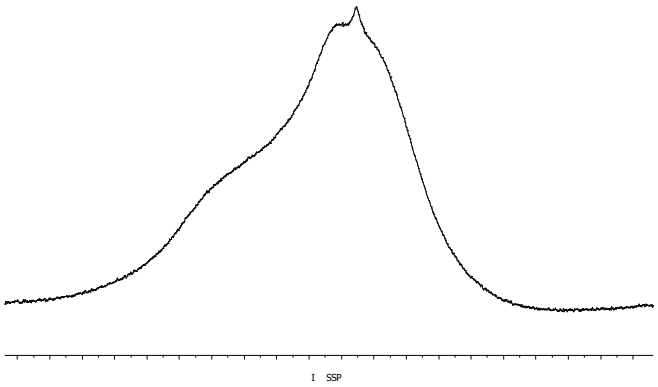
C_6F_5),
–159.8 (2F, *p*-C_6F_5), –164.9 (4F, *m*-C_6F_5). m. p.: 145 °C. IR (KBr) ν [cm^{-1}] = 2977 (m), 2929 (m), 2337 (m), 1694 (vs), 1644 (s), 1603 (s), 1559 (m), 1517 (m), 1464 (m), 1381 (w), 1277 (vs), 1248 (vs), 1099 (s), 1034 (w), 956 (s), 927 (m), 851 (s), 810 (s), 768 (m), 733 (m), 694 (s), 658 (w), 620 (m), 589 (m), 554 (s).

X-ray crystal structure analysis for (**3**). formula $C_{33}H_{26}BF_{10}O_2P$, M = 686.32, colorless crystal 0.20 x 0.10 x 0.05 mm, a = 14.7987(12), b = 13.7596(9), c = 15.5471(11) Å, b = 104.334(4)°, V = 3067.2(4) $Å^3$, $?_{calc}$ = 1.486 g cm^{-3}, μ= 1.629 mm^{-1}, empirical absorption correction (0.736 ≤ T ≤ 0.923), Z = 4, monoclinic, space group $P2_1/n$ (No. 14), ?= 1.54178 Å, T = 223 K, ? and f scans, 23707 reflections collected (±h, ±k, ±l), [(sin?)/?] = 0.60 $Å^{-1}$, 5344 independent (R_{int} = 0.077) and 3738 observed reflections [$I \geq 2\,\sigma(I)$], 430 refined parameters, R = 0.059, wR^2 = 0.144, max. (min.)residual electron density 0.37 (-0.22) e $Å^{-3}$, hydrogen atoms calculated and refined as riding atoms.

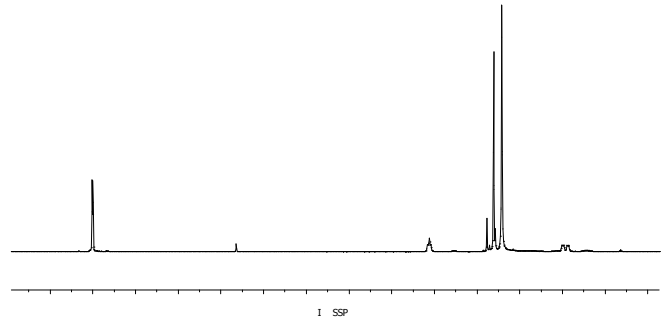




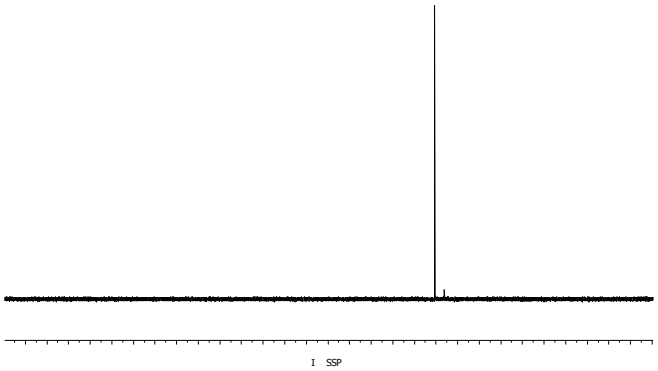
^{13}C {^1H} NMR (126 MHz, 223 K, $[D_2]CH_2Cl_2$) of (**3**).



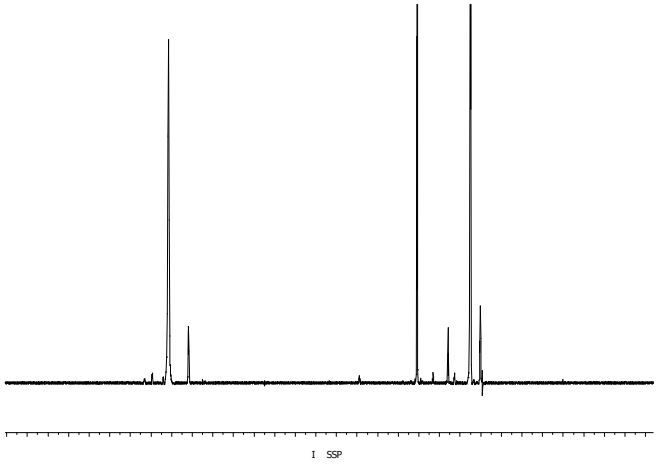
$^{11}B\{^1H\}$ NMR (160 MHz, 223 K, $[D_2]CH_2Cl_2$) of (**3**).



^1H NMR (500 MHz, 223 K, $[D_2]CH_2Cl_2$) of (**3**).



$^{31}P\{^1H\}$ NMR (202 MHz, 223 K, $[D_2]CH_2Cl_2$) of (**3**).



^{19}F NMR (470 MHz, 223 K, $[D_2]CH_2Cl_2$) of (**3**).

Comparison of Theoretical and Experimental Structural Data for 3

A comparison of experimental and theoretical data for important structural parameters of the CO_2 adduct of **2** is given in Table 1. In general the agreement between the experimental and theoretical data set can be regarded as very good. The largest deviation is observed for the rather weak P-C bond which is computed to be too long by 0.05 Å. The deviations for the other bond lengths are typically less than 0.03 Å and bond angles are computed in most cases with an accuracy of about 2-4 degrees.

Table 1. Comparison of experimental and calculated (B97-D/TZPP') structural data for **3**.
Bond lengths in Å, bond angles in degree.

Parameter	**3** (exp.)	**3** (calc.)
B-O	1.550	1.574
O-C3	1.284	1.283
C3-X	1.210	1.209
P-C3	1.900	1.954
C5-B-O	109.6	111.4
B-O-C3	130.9	132.5
O-C3-X	123.8	127.5
P-C3-X	116.8	116.2
C4-P-C3	102.5	104.1

Mechanism of the reaction of 2 with CO_2

The mechanism of the reaction of **2** with carbonyl-group containing molecules is investigated in an exemplary manner for CO_2. All relevant stationary point on the energy hypersurface have been computed at the B97-D/TZVPP' level (see Figure 1) and the relevant thermochemical data are given in Table 2. We first will discuss the energetic data and then include the thermal and entropic corrections that yield H(298) and G(298), respectively. As can be seen from Table 2, the two DFT methods provide similar results. The expected accuracy of the B2PLYP-D method for such relatively complicated bimolecular chemical reactions with not completely converged AO basis sets (due to the size of systems) is about 2-3 kcal/mol. As already noted in Ref.[1], the energetically favored form of **2** is a four-membered ring in which the Lewis-acid / base pair is "self-quenched". The B-P bond, however, is relatively weak so that an open form with a gauche conformation is only about 14.8 kcal/mol (B2PLYP-D/TZVPP') higher in energy and 13.0 kcal/mol using B2PLYP-D/QZVP(-g, -f), repectively. These compares very well with the recently determined experimental activation barrier for this process of 15.9 kcal/mol[2]. The corresponding value with the B97-D/TZVPP' functional is substantially lower (9.5 kcal/mol) which is similar to the value of about 7 kcal/mol previously reported in Ref.[1] with B97-D (but a slightly smaller AO basis set). The smaller values with the semi-local B97-D method compared to those with B2PLYP-D are attributed to the more approximate character of the former approach. Part of the rather large variations of the relative energies with the chosen density functional (and also the sensitivity with respect to the AO basis set) can be explained with the size of the systems and the non-covalent interactions between the bulky substituents that are in datailed balance with e.g. the P-B/CO_2 interactions.

2(open) is the active species that first forms a typical van der Waals complex with CO_2 (binding energy of 5.4 kcal/mol (B2PLYP-D/QZVP(-g, -f)). In this complex (**3**(vdW)), the CO_2 molecule is already located in the "bay region" between the P and B atoms of **2** but is closer to the P-fragment (P···C distance of 3.6 Å) than to the boron atom (B···O distance of 4.1 Å). We interpret this as some kind of lone-pair (P) carbonyl carbon donor-acceptor interaction. The orientation of CO_2 changes when going to the transition state of the reaction (**3**(TS), see Figure 1 and 2) which lies only 7.7 kcal/mol above **3**(vdW). This value corresponds to the intrinsic forward barrier of the reaction. The two P-C and B-O bonds are formed in a very synchronous and concerted manner as indicated by covalent bond orders of about 0.23 in the TS and similar differences of the P-C and B-O bond lengths to the corresponding values in the product (**3**) of about 0.6-0.7 Å. These values, the two C=O distances and the large bending angle in CO_2 (151 deg.) indicate the TS as rather "early". The overall reaction is almost

thermo-neutral (+0.9 kcal/mol (B97-D/TZVPP'), -1.3 kcal/mol (B2PLYP-D/TZVPP') and -2.9 kcal/mol (B2PLYP-D/QZVP(-g, -f)) at the three levels). The computed energy barriers for the decomposition of **3** back to CO_2 and **2** are 12.9, 18.1 and 18.2 kcal/mol, respectively, at the three levels which are in qualitative agreement with the experimentally observed thermal instability of **3** at 240 K. The corresponding data for the $P(tBu)_3$ / $B(C_6F_5)_3$ / CO_2 system are also given in Table 2. Here the overall reaction is much more exothermic while the "preparation" step (formation of **2**(open) or dissociation of the "frustrated" pair) requires almost the same amount of energy (13.0 and 15.6 kcal/mol, respectively).

Furthermore we tried to set up a model system for which high-level coupled-cluster calculations could be performed in order to benchmark the two DFT approaches. Unfortunately, this was not successful. When replacing the Mes / C_6F_5 substituents in optimized structures of **1** or **3** by hydrogen atoms, this PH_3-CO_2-BH_3 system dissociates without any barrier in geometry optimizations (at DFT and SCS-MP2 theoretical levels) to a complex of H_3PO and CO-BH_3. Although this prevents any reasonable calibration work, the result seems rather interesting as it emphasizes the importance of the bulky substituents for this (and probably similar) reactions.

The computed corrections to H(298) and G(298) are typical for mono- and bi-molecular reactions. The differences between energies and enthalpies are negligible in all cases so that the conclusions stated above remain valid when the more appropriate enthalpies are considered. The picture, however, changes considerably (as expected) for the bi- and trimolecular reactions when the free enthalpies are discussed. **3** should not exist under equilibrium conditions. The free enthalpy values, however, should be taken with some care because the large molecules have many very soft vibrational modes (<50 cm^{-1}) which may cause significant errors for entropies when treated in the harmonic approximation.

Table 2. Relative energies (kcal/mol) for stationary points on the **2** + CO_2 hypersurface at B97-D and B2PLYP-D theoretical levels (TZVPP' AO basis set); values in parentheses refer to a larger QZVP(-g, -f) AO basis. For comparison, total reaction energies for the reaction of $P(tBu)_3$ / $B(C_6F_5)_3$ with CO_2 and H_2 are also given. The B2PLYP-D values refer to B97-D optimized structures and the corresponding B97-D thermal and entropic corrections from a harmonic vibrational treatment.

reaction	? E B97-D	? E B2PLYP-D	? H(298) B2PLYP-D	? G(298) B2PLYP-D
2 → **2**(open)	9.5	14.8 (13.0)	14.2	8.0
2(open) + CO_2 → **3**(vdW)	-4.8	-5.9 (-5.4)	-4.3	4.5
3(vdW) → **3**(TS)	9.1	7.8 (7.7)	7.6	14.5
3 → **3**(TS)	12.9	18.1 (18.2)	17.5	15.8
2 + CO_2 → **3**	0.9	-1.3 (-2.9)	0.2	10.4
$P(tBu)_3$-$B(C_6F_5)_3$ → $P(tBu)_3$ + $B(C_6F_5)_3$ [a]	13.3	15.6	-	-
$P(tBu)_3$-$B(C_6F_5)_3$ + CO_2 → **1**	-9.0	-19.3	-	-
$P(tBu)_3$ + $B(C_6F_5)_3$ + CO_2 → **1**	-22.3	-35.0	-	-
$P(tBu)_3$ + $B(C_6F_5)_3$ + H_2 → **4** [b]	-30.3	-37.6	-	-

[a] A value of 11.5 kcal/mol has been reported at the SCS-MP2/cc-pVTZ level of theory for this reaction[3].
[b] A value of -26.3 kcal/mol has been reported at the SCS-MP2/cc-pVTZ level of theory for this reaction[3].

Theoretical Methods and Technical Details of the Computations

The quantum chemical calculations have been performed with slightly modified versions of the TURBOMOLE suite of programs.[4] As Gaussian AO basis, large triple-zeta (denoted here as TZVPP') sets of Ahlrichs et al.[5] have been employed. In standard notation these are [5*s*3*p*1*d*] for C, N and F and [3*s*1*p*] for H. For the reactive "core" of the systems (B and P atoms, C and O atoms of the carbonyl groups) the bigger TZVPP' basis set (2*d*1*f* set of polarization functions) is used. All geometries have been fully optimized at the DFT level using the B97-D semi-local GGA density functional[6] that also includes an empirical correction for London dispersion (also called van der Waals) interactions[6,7]. For a detailed description of this dispersion correction, that is of great importance in studies of large molecules, including many illustrative

examples see ref.[1,7,8] The theoretical level employed for structure optimizations is denoted B97-D/TZVPP'. It has been used successfully already (but with a slightly smaller AO basis set) to explore the reaction of **2** with dihyrogen[1]. In all DFT treatments, the RI-approximation has been used[9] for the Coulomb integrals which speeds the computations up significantly without any significant loss of accuracy. In passing it is noted that even according to present day computer resources the considered systems (up to 47 non-hydrogen and 73 total number of atoms) are rather large when extended basis sets are used (as we do).
The structures were used in subsequent single-point computations with the dispersion-corrected double-hybrid density functional B2PLYP-D[10,11]. This method (in addition to a portion of HF-exchange) includes a non-local correlation term that is derived from a second-order perturbation theory. The B2PLYP-D method (that also includes the London-dispersion correction) when used together with large AO basis sets is currently the most accurate DFT method for general thermochemical applications (see e.g. Ref.[12,13,14]). In these calculations we employ the huge quadruple-zeta sets (def2-QZVP[13]) with discarded g- and f-functions on carbon/fluorine and hydrogen, respectively. In standard notation they are then [7s4p3d2f]] for C and F, [7s4p3d2f1g] for B, [9s6p4d2f1g] for P and [4s3p2d] for H (denoted as QZVP(-g,-f)). In the perturbation treatments also the RI-approximation using corresponding optimized auxiliary basis sets[15] have been used. Analysis of the bonding situations was performed using Wibergs's covalent bond orders[16] and with the help of localised molecular orbitals (LMO) that both have been obtained from the Kohn-Sham determinants. The LMO have been computed using the localization algorithm of Pipek and Mezey[17]. All stationary points have been characterized as minima or transition states, respectively, by parallel calculation of harmonic vibrational frequencies (B97-D, unscaled) using the numerical derivatives of analytical gradients using the program SNF[18].

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Figure 1: Reaction mechanism for CO_2 fixation yielding **3**. The values refer to relative energies at the B2PLYP-D/QZVP(-g, -f)//B97-D/TZVPP' level..

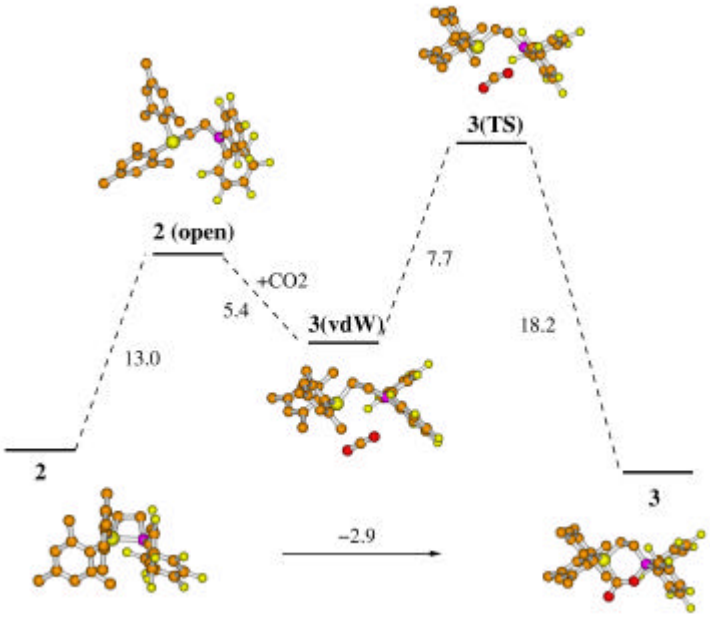
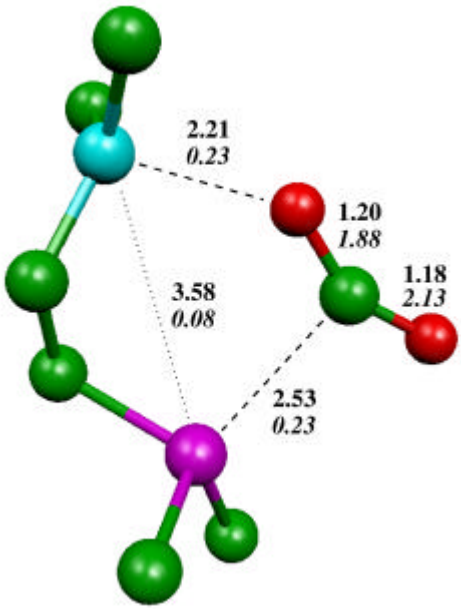


Figure 2: Structure of the transition state **3**(TS) with distances in Å and covalent bond orders written in italics. Atoms of the mesityl and C_6F_6 rings are not shown.



Optimized Structures

Cartesian Coordinates (B97-D/TZVPP') in Bohr

3

3.8672993628	0.1282646897	0.0263237150	p
-2.2943931953	0.1990408708	0.2637418170	b
-0.8170937838	0.0110568999	-2.3101515957	o
2.5083110713	-0.2225378229	-4.9088449759	o
1.8951799299	-0.7277306638	2.7531197743	c
1.3090593375	-2.6989507547	2.6136193761	h
2.9960984584	-0.4726965477	4.4887390778	h
-0.4236744056	1.0392391797	2.5803671268	c
0.2112408994	3.0068360513	2.4891927114	h
-1.4674462523	0.8762157089	4.3649700546	h
1.5486626173	-0.0260288389	-2.8435017150	c
6.5468399602	-1.8597587504	-0.8662529239	c
6.8861265816	-4.3452701622	0.0879336193	c
8.9924937831	-5.7308265629	-0.7111554116	c
9.2476406337	-7.6341707889	0.0294716311	h
10.7581866783	-4.7714439127	-2.4222739489	c
10.3773675290	-2.3280559768	-3.3416305194	c
11.7228315218	-1.5416144354	-4.6864547690	h
8.3133747468	-0.8390804417	-2.6209029819	c
5.1194077917	-5.6295339340	1.9342408985	c
3.2334470037	-5.8887452970	1.1192139200	h
4.9201685822	-4.5550958340	3.6941696020	h
5.8522911124	-7.5023264223	2.4208810717	h
12.9620432279	-6.3498919029	-3.3047824372	c
12.4529040975	-7.4013201065	-5.0242525316	h
13.5185412096	-7.7340785568	-1.8662042573	h
14.5999796105	-5.1640439940	-3.7607355773	h
8.1665299118	1.7907102230	-3.7447869626	c
8.8189605598	3.2196362317	-2.3908813748	h
6.2476991767	2.2826702524	-4.3275591222	h
9.3767109123	1.8921126918	-5.4217393247	h
5.0272134197	3.2909610161	0.8457030800	c
7.0136487987	3.4280684498	2.6465341224	c
7.8971297572	5.8143978465	3.3746610821	c
9.4185338688	5.9157394505	4.7579163027	h
6.8938579270	8.0504429282	2.3975866187	c
4.9390221457	7.8591537891	0.6317652829	c
4.1229975667	9.5786061338	-0.1514019203	h
3.9676896225	5.5347401941	-0.1733048646	c
8.3226500398	1.1538103878	3.7995197667	c
9.3603367022	1.7302599915	5.4960668174	h
9.6712148493	0.3181014964	2.4644295150	h
7.0125818839	-0.3537133641	4.3428678823	h
7.8423472404	10.5976566398	3.2594242207	c
9.7043935906	10.4432982891	4.1547844239	h
6.5352880955	11.4270515526	4.6461862899	h
7.9764744435	11.9211781021	1.6686498881	h

1.8571323844	5.5827121608	-2.0964047966	c
1.3458149115	7.5390410756	-2.5343687643	h
0.1567740155	4.6315787048	-1.4028794234	h
2.4131958200	4.6617293661	-3.8684346405	h
-4.6075036127	2.1537209682	-0.4657090166	c
-6.3022780614	1.4845221806	-2.3915877478	c
-6.0506115264	-0.7594085908	-3.5901695367	f
-8.3073060494	3.0134189640	-3.1737513508	c
-9.8755958900	2.2770968809	-5.0366718061	f
-8.6883875742	5.3423386186	-1.9909315756	c
-10.6009954416	6.8486833418	-2.7117229728	f
-7.0603925371	6.0906518742	-0.0570349546	c
-7.4173795659	8.3359718498	1.0927198677	f
-5.0800352937	4.4935729423	0.6638690008	c
-3.6000352908	5.3575195230	2.5778800032	f
-3.4106671128	-2.6430455784	0.9713016590	c
-5.3556285645	-2.8569984781	2.7522824612	c
-6.3367199851	-0.7442179450	3.8267147232	f
-6.3789673779	-5.1578197225	3.5459271581	c
-8.2630542348	-5.2394905158	5.2527163213	f
-5.3985570294	-7.4070490271	2.5722349922	c
-6.3290927010	-9.6466563222	3.3240882126	f
-3.4202924640	-7.3007235684	0.8321203896	c
-2.4231495211	-9.4604217663	-0.0789556853	f
-2.4735729839	-4.9477574494	0.0868974854	c
-0.4865081954	-5.0219085521	-1.5531748187	f

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2 (quenched)

0.1069819403	2.5607227951	-1.3831171478	p
-0.9399143266	-1.4395784146	-2.0368533778	b
-0.8724361484	2.4918281317	-4.7354493676	c
-0.8729526239	-0.4331932200	-5.0090076171	c
-1.1834568305	5.3883934842	0.2049127659	c
-0.4108498156	7.8170040991	-0.6519441816	c
-1.4344521061	9.9659899036	0.4889637382	c
-3.2025802811	9.8079129879	2.4532139149	c
-3.9188369003	7.4108721821	3.2761960137	c
-2.9464128125	5.1885970151	2.2021194428	c
3.5651110047	2.5546807146	-0.8668106271	c
5.4329318829	2.4905890763	-2.7964094312	c
7.9483935060	1.9961661510	-2.1270925852	c
8.7117131901	1.5787782833	0.3607387916	c
6.8762283483	1.7750869715	2.2438784324	c
4.3366130708	2.2520162137	1.6937281360	c
-3.7405873837	-2.4192186405	-1.2404094951	c
-5.8977493318	-0.8882335621	-1.2777658647	c
-8.3317137039	-1.7386508783	-0.7193381501	c
-8.7100626063	-4.2914252243	-0.1761993390	c
-6.6389819673	-5.9253543142	-0.1884335872	c
-4.2343544195	-4.9782691324	-0.7386812641	c
1.4224227914	-2.9011027955	-0.7213065991	c
3.7211957852	-3.4760359796	-1.9038584856	c
5.8587893838	-4.3376125469	-0.6120876580	c

5.7512811350	-4.6948148699	1.9927347435	c
3.4857054254	-4.2267766756	3.2570481647	c
1.4055258337	-3.3717847660	1.8893401260	c
1.4876875645	8.1779370772	-2.7570197179	c
-4.3210052254	12.1669363565	3.6043348417	c
-3.8397697529	2.7284687169	3.3499292497	c
4.9354171988	2.9509593322	-5.5736045487	c
11.4013461139	0.8713934897	0.9835105924	c
2.5416498693	2.4525588095	3.9067141537	c
-5.6909984145	1.6111490729	-1.8348540522	f
-10.3082540950	-0.1348152657	-0.7177542511	f
-11.0344339544	-5.1633983751	0.3439429253	f
-6.9870363808	-8.3954841822	0.2999030941	f
-2.3423836820	-6.6980874130	-0.7746738328	f
4.0177856124	-3.1949853515	-4.4327495228	f
8.0387194573	-4.7785987758	-1.8494065147	f
7.8089939901	-5.4484675646	3.2750283971	f
3.3603286424	-4.5368934058	5.7803494858	f
-0.7141667140	-2.8987151786	3.2606802344	f
0.2264761159	3.5529517966	-6.1148772784	h
-2.7962722712	3.2461105710	-4.7262285287	h
0.7877471122	-1.0657704219	-6.0521612231	h
-2.5354482952	-1.0707755285	-6.0722924805	h
-0.8295958149	11.8185717698	-0.1771949454	h
-5.2772372980	7.2421832135	4.8154469509	h
9.3564173782	1.9157003497	-3.6262754405	h
7.4197259286	1.5114107224	4.2119493688	h
1.8337402087	10.1931807685	-3.0811568097	h
0.8057679325	7.3546737962	-4.5337274963	h
3.2922373772	7.2645969568	-2.3057610305	h
-5.1641972664	11.7709901805	5.4551552883	h
-2.8813875608	13.6426624004	3.8335110750	h
-5.8124434930	12.9407171438	2.3804844951	h
-3.2437457465	2.6207173358	5.3352658167	h
-3.1135780603	1.0619864524	2.3857999213	h
-5.9105298343	2.6413066580	3.3142808102	h
6.7256964817	2.9578772818	-6.6121969308	h
3.7439028341	1.4806821049	-6.4058895574	h
4.0195484473	4.7813479991	-5.8829655499	h
11.9236749875	1.5024214855	2.8875667608	h
12.7291522878	1.6920450232	-0.3805927715	h
11.6312775131	-1.1930648121	0.9187959566	h
3.4587645434	1.7765710353	5.6351146079	h
1.9452276016	4.4166776576	4.2013658713	h
0.8247769637	1.3388690556	3.6389337897	h

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2 + CO_2 (TS)

-4.89674379946670	-4.60200201017860	0.00059288462598	c
-4.24832277883402	-2.16458519642101	0.93812437356064	c
-6.11263407397344	-0.72514918387835	2.22164859407906	c
-8.51751754266611	-1.76895543354513	2.58732157508988	c
-9.17297027770487	-4.17393699680854	1.71930680038893	c
-7.32811397296009	-5.55147518886448	0.43222694396189	c

-1.02337780485028	-1.10076317437437	0.15650775496886	p
1.15480080241847	-3.43797260497702	1.60418851081012	c
0.82827709823006	-4.27484488911283	4.12972560068044	c
2.57671329104041	-5.98579398331353	5.14815695729569	c
4.63162118251923	-6.89653014405838	3.76487129407981	c
4.90934306902801	-6.06414484435860	1.27288467560084	c
3.21629992485550	-4.36255725330174	0.16102306104237	c
-1.35932766445893	-3.48776074712662	5.79731415019950	c
6.52390706784570	-8.68499218175709	4.93232073312878	c
3.66166657965981	-3.62579219257596	-2.56707077383962	c
-5.67763300554199	1.90431783840242	3.25890935688598	c
-11.80438785895493	-5.21167693422295	2.09144252038775	c
-3.06815493559755	-6.27600650083628	-1.43093585954474	c
-0.84346982327520	0.10198447644168	-4.45797335159286	c
-2.38104220178131	-1.17504154329666	-5.45438334856917	o
0.76441006107222	1.70710611894078	-4.51014599459760	o
0.04605142490172	1.81136292333227	1.83367380689425	c
2.62114326183356	2.57933413954027	0.68712099165324	c
2.58490395786721	4.28320442375479	-1.78108275630807	b
5.01742338351426	4.52803830856415	-3.54965897993921	c
4.83726543214022	5.57058066195566	-5.98701786728193	c
6.89589348930817	5.79392612425233	-7.62048934964899	c
9.27914660695064	4.99202050985035	-6.81111534205002	c
9.56030807329698	3.96843563211047	-4.39532354715557	c
7.44791982107152	3.75858926709161	-2.82369546875067	c
2.59239590904668	6.39270144327719	-6.86893164311597	f
6.62333210102587	6.77751777510251	-9.94443812839962	f
11.28185736729197	5.20589057103403	-8.34371704850604	f
11.85387429426850	3.21315214863787	-3.60669929324610	f
7.87241371983747	2.79628676147985	-0.49452637754053	f
0.67468631567638	6.65883025911988	-1.76560574397797	c
-1.95547824014661	6.62440531569471	-2.03754616447692	c
-3.45706830266268	8.79436018045905	-1.90174316356876	c
-2.32698235301558	11.13130363571954	-1.43079449356378	c
0.28953383938637	11.26073254268977	-1.10706354368425	c
1.71606767586211	9.04707793625402	-1.27126794729842	c
-3.20988042172255	4.43100620204448	-2.46188185804340	f
4.23878566098400	9.27956284355360	-0.88497706889794	f
1.39327723388914	13.49386687149968	-0.62155562327946	f
-3.74091830624031	13.22600111564441	-1.26953519077627	f
-5.97648345810894	8.64851712424814	-2.18825505026761	f
-1.33088939106449	3.32177695103848	1.60144941850777	h
0.24165545344318	1.42333588271020	3.85714044683150	h
3.85268370850455	0.92594355550479	0.51756506677256	h
3.58857385631075	3.79911969667599	2.08027509821750	h
-9.92590665324455	-0.65213248437409	3.59267061730496	h
-7.78783241370895	-7.42716119694213	-0.28313083111109	h
-5.31949995417117	3.26511376353641	1.73791745832294	h
-4.06975560557205	1.96994099386223	4.56233668366875	h
-7.35416661130143	2.54580295067503	4.29036944244146	h
-13.01983122845596	-4.72039012068543	0.47771145080032	h
-12.68483122512858	-4.42841816190641	3.79730367008828	h
-11.78034560317850	-7.27906602345316	2.24705781270220	h
-1.62350983674794	-7.07275347421962	-0.17504189350013	h
-2.08791040687633	-5.22882335332499	-2.92547555649694	h

-4.09106783062313	-7.84128071055684	-2.32123917320666	h
2.31555890443438	-6.61988330940065	7.09039589148621	h
6.48764104210595	-6.76128940085990	0.14887408865885	h
-0.93364923349051	-3.91836253272912	7.77837979237295	h
-3.09207933545732	-4.49626676724768	5.26774284412534	h
-1.79068083712595	-1.47115317585627	5.64962188757681	h
5.72523711290130	-9.64995180255378	6.58338710271709	h
8.21582496258396	-7.65246467431025	5.55917930542588	h
7.14392002563145	-10.11536245970963	3.56444627959073	h
5.33803110242372	-4.59154111439790	-3.30548225205847	h
3.94577574087728	-1.58783850005511	-2.78680052739823	h
2.04424243407025	-4.14702667910804	-3.75658373125246	h

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2 + CO_2 (vdW)

1.8064868636	9.2385554592	-0.1714728425	c
0.9004829705	6.9032540634	-0.9968412174	c
-1.6297778445	6.8242669382	-1.7261358197	c
-3.2043510660	8.9411697385	-1.6460204634	c
-2.2268067133	11.2470560453	-0.8005630146	c
0.3048271450	11.4064647124	-0.0596311910	c
2.7812797011	4.5378279279	-0.8760257924	b
4.6286474495	4.0456245108	-3.1454202815	c
3.9649339218	4.6069501887	-5.6635529521	c
5.5152725279	4.0432571910	-7.7194392622	c
7.8734712137	2.9314570364	-7.2902464454	c
8.6451139037	2.3871612101	-4.8213266567	c
7.0310016917	2.9436930118	-2.8149933553	c
1.7085645642	5.6500893507	-6.1998492248	f
4.7771320447	4.5467478142	-10.0902902107	f
9.3894981138	2.3894177149	-9.2354128701	f
10.9173415194	1.3346353755	-4.4183197687	f
7.8927110000	2.4103158625	-0.4811247693	f
-2.6328641346	4.6322157702	-2.5768015250	f
-5.6340138291	8.7861244942	-2.3624272233	f
-3.7111758553	13.2977124347	-0.7019741099	f
1.2514472144	13.6160048154	0.7530776167	f
4.2545668587	9.4288341865	0.5740116200	f
0.2270341591	-0.1109631531	-6.9610383838	o
-1.9192209573	-0.0777128015	-6.4370102466	c
-4.0733618534	-0.0619727086	-5.9744145077	o
2.8030348427	3.0376481650	1.7061604412	c
0.1315737124	2.1249723824	2.4834925069	c
-0.6705049551	-0.5537707757	0.2659447360	p
1.4173872132	-2.9924695391	1.7407295879	c
0.9375574992	-4.0384526655	4.1644461086	c
2.6642644354	-5.7668824972	5.1890881762	c
4.8516291915	-6.5078063557	3.9078461287	c
5.2742680288	-5.4953866163	1.5073925673	c
3.5991386784	-3.7721198842	0.3945133794	c
-1.4155154186	-3.4879993525	5.6980348947	c
6.7197248712	-8.3063469138	5.1005842167	c
4.1702350682	-2.9165870588	-2.2760817932	c
-3.9069702980	-1.8212391221	0.7713571406	c

-4.3876594386	-4.2113298775	-0.3660666617	c
-6.7956668158	-5.2932480158	-0.1779337158	c
-8.7909343114	-4.0858845068	1.0525564449	c
-8.3153042522	-1.7055456504	2.0895469571	c
-5.9410455376	-0.5415303257	1.9625103635	c
-2.4000160501	-5.6990150612	-1.7915777769	c
-5.7160885522	2.0581129460	3.1341574916	c
-11.3888435183	-5.2614202344	1.1759936399	c
-1.2230528136	3.6606608442	2.2504847377	h
0.1188621128	1.5402283737	4.4685748728	h
4.1291540450	1.4537561021	1.7579923386	h
3.4527348791	4.4015718541	3.1509445314	h
-9.8470215431	-0.7046597885	3.0360963387	h
-7.1139131297	-7.1352297422	-1.0441113988	h
-5.1861104115	3.4771171287	1.7185945775	h
-4.3002163028	2.1103001714	4.6449511560	h
-7.5314221782	2.6324857898	3.9482559022	h
-12.5383093124	-4.6833431602	-0.4575553402	h
-12.3984785907	-4.6695949591	2.8881233636	h
-11.2760125998	-7.3318399511	1.1587036991	h
-1.0420996939	-6.5929399275	-0.5047245933	h
-1.2969155493	-4.4870630287	-3.0651977963	h
-3.2979594065	-7.1805959294	-2.9276048107	h
2.2782692216	-6.5572649761	7.0524098339	h
6.9508868346	-6.0650950903	0.4550744818	h
-1.1201519652	-4.0287021939	7.6766965404	h
-3.0303585880	-4.5630462814	4.9634341220	h
-1.9738587731	-1.5007365311	5.6376796230	h
5.7738368470	-9.6187476557	6.3977398897	h
8.1460330053	-7.2630583794	6.1963555713	h
7.7242004848	-9.4079867013	3.6596003079	h
6.1460343576	-3.3194342077	-2.7540729070	h
3.8113861188	-0.9049721974	-2.5619773529	h
2.9659779484	-3.9236957927	-3.6359196252	h

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2 (open)

2.6997318768	7.1783996768	0.3815243243	c
1.6894809081	4.7862440634	-0.1007365708	c
-0.8636526692	4.7117350509	-0.7575959811	c
-2.3510403571	6.8876655844	-0.9316358526	c
-1.2697020839	9.2445382329	-0.4227792575	c
1.2840428885	9.4001491438	0.2387683677	c
3.5487753379	2.4265276045	0.2264118892	b
5.5453438722	1.9238929942	-1.9179079619	c
4.9407054107	2.1803823517	-4.4943804492	c
6.6463875920	1.6239167195	-6.4277486392	c
9.0899248185	0.8325928997	-5.8023522632	c
9.7928455280	0.5922639378	-3.2652774161	c
8.0240468453	1.1235932335	-1.3855007884	c
2.6023723978	2.9002116529	-5.1940679565	f
5.9799748978	1.8372409996	-8.8645066787	f
10.7550622564	0.3085496940	-7.6287822402	f
12.1463916160	-0.1472904561	-2.6777571674	f

8.8031067239	0.8857170367	1.0264734662	f
-1.9773510426	2.4815922762	-1.3055968019	f
-4.8012539418	6.7390205112	-1.5782208432	f
-2.6749948980	11.3472200632	-0.5698220189	f
2.3324026608	11.6576588752	0.7333463121	f
5.1727456278	7.3720426891	1.0402603222	f
3.5300603190	0.9846043905	2.8365473194	c
0.8669867345	0.0572258450	3.6055085444	c
0.0755295485	-2.6036967014	1.3620066925	p
2.2157716092	-5.0537858577	2.7451726373	c
1.8220843857	-6.1474694094	5.1617960586	c
3.5888516864	-7.8886175917	6.0959102530	c
5.7285725218	-8.6041941121	4.7247036689	c
6.0609387229	-7.5536821737	2.3250186067	c
4.3470668480	-5.8122636403	1.3056300948	c
-0.4833228386	-5.6406354310	6.7799798229	c
7.6406359392	-10.4215157318	5.8144993794	c
4.8194127178	-4.8963185141	-1.3654031668	c
-3.1361397189	-3.9187908388	1.9390794859	c
-3.6279662460	-6.2876874393	0.7606481452	c
-5.9986348665	-7.4310005453	1.0463307064	c
-7.9531330736	-6.3005937999	2.4081108357	c
-7.4780223541	-3.9318125774	3.4722805352	c
-5.1387509423	-2.7106068947	3.2555651326	c
-1.6894422091	-7.6789587793	-0.8207093673	c
-4.9200282509	-0.1306666299	4.4732007041	c
-10.5133897244	-7.5405285372	2.6415288925	c
-0.4936630285	1.5870598200	3.3643798730	h
0.8507366085	-0.5240242825	5.5913748719	h
4.8784984922	-0.5811565133	2.9244726546	h
4.1588424565	2.3819488918	4.2594883641	h
-8.9821165809	-2.9875021751	4.5162707150	h
-6.3203425507	-9.2585268627	0.1514422068	h
-4.4655415283	1.3268614050	3.0704723344	h
-3.4544080544	-0.0803766533	5.9357772844	h
-6.7168775840	0.3918398797	5.3612619981	h
-11.7783324931	-6.9166885827	1.1134713089	h
-11.4227560403	-7.0497455172	4.4398199393	h
-10.3596107226	-9.6047296454	2.5217337143	h
-0.2072032180	-8.5317536899	0.3515547254	h
-0.7442522677	-6.3976893307	-2.1536113987	h
-2.6053920570	-9.1838681882	-1.9109614165	h
3.2698172138	-8.7134073355	7.9568176338	h
7.6935400246	-8.1114169175	1.1998194793	h
-0.1230408585	-6.2183748397	8.7373912149	h
-2.1140133484	-6.7118554677	6.0750178184	h
-1.0541308431	-3.6564757185	6.7761086265	h
6.7561749293	-11.7186675073	7.1687343671	h
9.1411277203	-9.3922623499	6.8208172766	h
8.5470335262	-11.5394864529	4.3217061383	h
6.6849685850	-5.5183040150	-2.0202133127	h
4.7165783320	-2.8398794030	-1.5191599582	h
3.3899362132	-5.6583884143	-2.6645072356	h

CO_2

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0.00000000000000	0.00000000000000	-2.20694422598071	o

$B(C_6F_5)_3$-$P(tBu)_3$ complex

4.69380271268846	-0.62915139247811	1.31906598648337	b
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-2.44840775823672	0.33030229863866	-0.68862406412380	p
-2.77657065990608	1.31765829719232	-4.20607491245710	c
9.58546634465406	-1.53918586332885	-6.70513931825551	f
-0.83335419129064	-0.26907972334038	-5.71319354358897	c
7.87167400251518	3.01904423836283	-8.43316912868058	f
-1.95770969810455	4.09797290497311	-4.55672318387001	c
4.75288893831121	5.90258864214149	-5.48848411186360	f
-5.40830736174965	1.01382455775399	-5.41748724955062	c
3.37684641454128	4.28609505805871	-0.87785877026117	f
-4.43442189300523	-2.72532714728739	-0.26926847025967	c
7.86293257091153	3.79679152397144	2.41094857078023	f
-3.76572422355491	-4.66078744887626	-2.35006230460135	c
7.09072521282683	7.08234444098975	6.21333177407298	f
-3.57762856011137	-3.95080768525425	2.24665902623498	c
3.22307552230628	6.33327429976608	9.55762561191556	f
-7.33116236278655	-2.41890189121949	-0.24840528090103	c
0.13071364559559	2.22162452689902	9.06699422062647	f
-4.10825169130542	2.93685600549727	1.28873557241914	c
0.88932875587953	-1.11379183249424	5.31683534424822	f
-2.17397428778315	5.10871786774133	1.61630949332267	c
5.93211605561387	-3.51691776057845	5.89387205451255	f
-6.59198046959781	4.01897400728773	0.21819582264490	c
4.96012233648285	-8.45879160332467	6.58869347482565	f
-4.65821349954159	1.96439793711537	3.98585631870202	c
2.82346783310394	-11.25035668097767	2.80167693589701	f
5.63502044831985	0.40512420290347	-1.31272599913583	c
1.68659632108092	-9.03623780074345	-1.72799885355464	f
7.26846025401289	-0.98179011305215	-2.88643620907794	c
2.68638542286424	-4.11681093299337	-2.48990416184292	f
8.02939770861568	-0.14639446258434	-5.26801113300870	c
7.16780285238751	2.18917215949400	-6.15407125065768	c
5.57616861840758	3.65823346428809	-4.64111789152355	c
4.88693506324234	2.77301462311375	-2.25824978795229	c
4.34660882127516	1.23444075265110	3.61877070943916	c
5.90590002079565	3.35628971092674	3.98256996422449	c
5.55781225732192	5.08117737031588	5.94536028316724	c
3.59042261173232	4.69885613363774	7.66736121561072	c
2.01600441157840	2.59285061993663	7.41123288834807	c
2.44773297029667	0.89408238669657	5.44562685887011	c
4.26059000624210	-3.55347454371201	1.69916320968502	c
4.84487207402726	-4.79502725845380	3.97569931934009	c
4.37510909617800	-7.35684481277976	4.38188987643240	c
3.29410643208903	-8.79446717108429	2.44615120849130	c

2.71866746101275	-7.65550413181896	0.13262374189119	c
3.25084224143574	-5.09914445501349	-0.21118170914985	c
1.07974582258495	0.01007980173009	-4.97175922984735	h
-1.23873168156609	-2.29025001408155	-5.68569341948989	h
-0.86445717080514	0.36521739663373	-7.69350623211028	h
-0.11958371118179	4.48044414139695	-3.69878225071302	h
-1.79734046549722	4.46596898062989	-6.59610201150367	h
-3.32815315887612	5.44047896530419	-3.79306713535192	h
-6.02138808761063	-0.95664761815218	-5.49902424909819	h
-6.85108978629896	2.10142292306278	-4.41451424307064	h
-5.31863670505612	1.71764529076820	-7.37355481574554	h
-1.72877826643706	-4.94922727965494	-2.51690313214392	h
-4.62590821398334	-6.48057028725317	-1.83165788816444	h
-4.50632120725622	-4.13376368921446	-4.20412330643217	h
-1.53826971322320	-4.30916670762567	2.23544084996228	h
-4.01303708349973	-2.80012931312944	3.90102818562102	h
-4.55862470797852	-5.77258234235413	2.45533812328104	h
-8.03024937888308	-1.56001811989716	-1.99314946449980	h
-8.19224045933319	-4.30502214391348	-0.07250209154546	h
-7.99818145665289	-1.28625425484951	1.34464022745439	h
-1.67609840060888	6.02813796431244	-0.16062419221273	h
-3.00660446259759	6.54376915999774	2.87019760642446	h
-0.42894167140448	4.41657035616884	2.48972252270346	h
-6.32085774548970	4.99691153813666	-1.58021124076527	h
-8.02291169164583	2.55205791519061	-0.04976904479715	h
-7.34428898283250	5.40764493399008	1.57319813082012	h
-6.19627875888396	0.58825195374529	4.04419286539352	h
-2.99135639535368	1.11972180054038	4.86214319981308	h
-5.23362649707028	3.58936531861646	5.14718073666574	h

1

3.95329593271867	-0.55551715893583	1.38209746392967	b
-0.08545200166622	1.35604954064442	-0.24354517646844	c
3.38254575995329	-3.85993136640240	-2.92984363136175	f
0.73407513906864	3.42177183409972	-0.79893320613296	o
-3.53978066252653	0.71153969843109	-1.16485982673788	p
-3.52594904970047	1.53457400594649	-4.68476054599080	c
4.88832534277303	-3.02955593266882	-7.70191916906069	f
1.00108800429679	-0.55108498691003	0.80701496487177	o
-1.13607127013684	0.38444346671610	-5.92308194921903	c
-1.22543005919269	0.83052326038952	-7.94774152681165	h
-0.99811576279516	-1.66147139353903	-5.73313909938298	h
0.58383808125568	1.24010508687277	-5.16403171174059	h
7.49664043178410	1.29189573036746	-8.91285210244505	f
-3.36940847597207	4.42277287922375	-5.09581230645034	c
-1.71765022930556	5.23676921245681	-4.16501191443170	h
-5.07316342407020	5.41244158754017	-4.47760017845415	h
-3.18242803901491	4.72007281347308	-7.14145866985286	h
8.50718287128979	4.78763917605053	-5.22953154137675	f
-5.91989693429249	0.55001444202565	-6.02520093754771	c
-7.65217265838692	1.30510544386555	-5.18463984172773	h
-6.03321303027943	-1.51095167658002	-6.05011387067467	h
-5.83267715480652	1.19634825062983	-7.99513719337847	h

6.96900224863768	4.04688936462912	-0.47868464021396	f
-4.51975773130300	-2.71776191195790	-0.60019550993085	c
8.99373108569606	0.27252944734872	3.03309013422012	f
-3.17328862029019	-4.45756344842179	-2.51916277474932	c
-3.63896014418435	-6.40935018879317	-1.99073329393750	h
-1.12103952324650	-4.24886129840184	-2.42387829288816	h
-3.81047067171739	-4.17322625222124	-4.46193055502453	h
10.61810967967643	3.19673781405865	6.88837226524801	f
-3.70878878344481	-3.65852452561806	2.04846212714732	c
-4.45826832834086	-5.58591311397378	2.23399371272578	h
-4.45792175476499	-2.54130357641068	3.60541377968788	h
-1.66259045363006	-3.73620838370643	2.21859066387424	h
7.21750470495959	5.94419090898326	9.68409997661855	f
-7.41012437745975	-3.03139518341754	-0.86122472364849	c
-8.14652891484322	-2.34185786472330	-2.66357122568417	h
-8.42916282220684	-2.10217217955746	0.67801408425823	h
-7.81638161321741	-5.06285512134677	-0.73948922175371	h
2.16640164004723	5.69039243349776	8.54326520236193	f
-5.53949207183974	3.01274720413562	0.75659208033959	c
0.50668367890517	2.79151803387383	4.77237800172345	f
-4.20240265697457	5.59976726066434	1.02233032837534	c
-5.51198301726946	6.82691542596745	2.06629862998790	h
-3.77831827282034	6.49544137869126	-0.78242074190945	h
-2.45410634434455	5.44268043558942	2.10570482910572	h
1.21513879586516	-2.73353712898696	5.61467907282799	f
-8.15568360889235	3.39646241374167	-0.47896721987008	c
-9.19434871336974	1.62627893588520	-0.71413302637841	h
-8.03057775996920	4.34129977631700	-2.31107428854657	h
-9.25774967983400	4.62001450591449	0.78411213470309	h
1.95393255639932	-7.26609898148659	7.79139275401948	f
-5.91375102052570	1.98265873057606	3.46295751667419	c
-6.84474289692311	3.47983398512449	4.55684556234091	h
-4.11502827810292	1.55111184999911	4.38669230983188	h
-7.13723085700015	0.31953725995186	3.51386134610044	h
5.76471281467608	-10.37386579125055	6.13423053836644	f
5.19740421410738	-0.00870719324587	-1.42127229272423	c
8.78433871659642	-8.85943533028590	2.21289200798924	f
4.70889804089101	-1.70385755454691	-3.39202385230483	c
8.04302525073184	-4.39810933743439	-0.04460643295124	f
5.45674510140477	-1.32915367253012	-5.88935379074679	c
6.76739927001682	0.87211980653149	-6.51683702541220	c
7.28308023013832	2.63961727230445	-4.63072873873023	c
6.47849265348409	2.18629809471986	-2.15022450820430	c
4.70056052484951	1.43871984190649	3.64887269202949	c
7.24892133647549	1.60602453185825	4.34806934783582	c
8.13954759976619	3.09491302677414	6.33126809270210	c
6.41587517919490	4.49598438750982	7.75890025594183	c
3.85252989310468	4.36470545623860	7.16546257397492	c
3.05374548173358	2.84030010918062	5.15885849537280	c
4.49539525852875	-3.38729043478274	2.57786315046773	c
3.06486922633706	-4.22827419461392	4.64135250087825	c
3.42640964047813	-6.55074253734045	5.83936176437019	c
5.36727988305778	-8.13285850032537	5.00962060017383	c
6.89476529071114	-7.35361016691194	3.00653695884981	c
6.44861610905075	-5.01670973337810	1.85017863492957	c

$P(tBu)_3$

1.56187067634903	0.18593743031183	0.45816721695993	p
1.01779914137781	1.11600172652826	-3.04823733928366	c
3.30514847132825	0.09623205622047	-4.56648484153458	c
3.16556762040651	0.79857797166796	-6.51963477208737	h
3.37885588901512	-1.96339602427730	-4.64300464657387	h
5.08783743531035	0.78070360803015	-3.75755196472324	h
1.15969903603540	4.02087380780691	-3.30516366458883	c
2.85099952183009	4.78433840077032	-2.38044633458859	h
-0.50503492343883	4.97319350703446	-2.53772088364804	h
1.26926858792523	4.48962639284400	-5.32791230190363	h
-1.44584061666218	0.21508152685436	-4.31094269220353	c
-3.12216280851976	0.88458391028925	-3.30348847297749	h
-1.54971663027303	-1.84478068364068	-4.44222760341912	h
-1.52009515219631	0.96609873393551	-6.25104081786510	h
0.41017991160719	-3.28004424479389	0.80474964236916	c
1.62906374090647	-4.91232656155833	-1.28687645743330	c
1.30315617789912	-6.91272176553205	-0.82285031642751	h
3.67718718038324	-4.60740055512463	-1.39276098772095	h
0.80770936475619	-4.56638051180065	-3.15041753239206	h
1.51585766985498	-4.29800438904162	3.31845486615425	c
1.08947908103549	-6.32984853693128	3.45119774027324	h
0.72487131197158	-3.37986391839472	4.98734300003893	h
3.57593947744969	-4.06373614735203	3.36287322048800	h
-2.46219312673504	-3.75316049866918	0.76248924004951	c
-3.33422094240267	-3.06611522174085	-0.98136243587701	h
-3.42556490861842	-2.86517826954914	2.36078801327476	h
-2.80752250008956	-5.80210515362790	0.88905714670751	h
-0.73018697846758	2.24685558340031	2.44806563279688	c
0.57136330642992	4.84235086607813	2.83033933219535	c
-0.57772779469312	5.96813735162155	4.14937642380355	h
0.76250216843206	5.92255745581926	1.08383732902874	h
2.45855768065369	4.60318934539972	3.65633834603831	h
-3.41357927436575	2.66849802719579	1.40017497133016	c
-4.41423672659609	0.88582013095438	1.09388779336367	h
-3.40294301374844	3.71838475662743	-0.38015666178318	h
-4.50331972149555	3.78881697273468	2.77525963806961	h
-0.97110057360854	1.10689390087534	5.12525984656917	c
-1.92473147149446	2.49864498038167	6.34059640757684	h
0.88784247247846	0.70607221178731	5.95121791396846	h
-2.10057876003043	-0.62240817313484	5.15880700597510	h

$B(C_6F_5)_3$

-4.70048236327400	-0.33884462496556	-1.40927788513901	c
-2.82220355753015	0.90044800653293	0.00361845693338	c
-3.62900978339058	2.99940957317372	1.41926367173773	c
-6.13417859419689	3.81643258569182	1.46439876646693	c
-7.93421632077469	2.53443217266643	0.01147755377425	c
-7.21568100900864	0.44691387359961	-1.44493163407921	c
0.00497328983309	-0.00398583211821	0.00076242364338	b

0.63722880003599	-2.90387329255354	0.00249834545028	c
2.65401899596237	-3.90805987756816	-1.40666649559509	c
3.22702717493654	-6.48000294860338	-1.45161232035762	c
1.77154483245638	-8.15022540608005	-0.00719571614706	c
-0.24217964387711	-7.23550862822147	1.44302528919649	c
-0.78293964680456	-4.65661826357674	1.40715614144575	c
4.09346401060984	-2.37764432187138	-2.84806807827207	f
5.14231116480788	-7.36874579786159	-2.85123901721039	f
2.30443499440106	-10.61677361039415	-0.01216820544980	f
-1.61848772639044	-8.84148077568595	2.83727585124353	f
-2.72646102194428	-3.86244475601986	2.85058763668185	f
-1.96787824159287	4.28011541246103	2.86649931458692	f
-6.83753017896988	5.80307923680877	2.86993076086545	f
-10.33808818678779	3.30265684671783	0.01551075285571	f
-8.94503804768292	-0.76317744825931	-2.84573891569755	f
-4.09306669477119	-2.34393623023448	-2.85973354144847	f
2.19813982598763	1.99583039425142	-0.00485777895041	c
2.06103492571582	4.23040751682263	-1.43535473961542	c
3.99235595521094	6.02287173088005	-1.47623952743943	c
6.15306554966920	5.62265563079255	-0.00440236920600	c
6.36555233571656	3.43467736128133	1.46627685762260	c
4.41346944918380	1.66455916250363	1.42369282674361	c
0.02596142917514	4.68661855606798	-2.89957125762560	f
3.80764797044464	8.11276854816363	-2.89587514527366	f
8.01189703001378	7.32949495935901	-0.00279073436355	f
8.43121676734910	3.07088361966324	2.88688069329317	f
4.69209651548613	-0.40293337342378	2.88686801932947	f