

Supporting Information for:

**Synthesis of a Mononuclear, Non-Square-Planar Chromium(II) Bis(alkoxide)
Complex and its Reactivity Toward Organic Carbonyls and CO₂**

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1. X-ray crystallographic details

Table S1. X-ray crystallographic details of HOR' and complexes **2**, **3**, **7**, and **8**.

complex	HOR'	2	3
formula	C ₂₇ H ₃₂ O	C ₆₂ H ₇₈ CrO ₄	C ₆₈ H ₇₄ CrO ₄ ×2C ₄ H ₁₀ O
fw	372.54	939.28	1007.31
crystal system	monoclinic	triclinic	triclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	12.9525(6)	13.2611(6)	14.3588(8)
<i>b</i> (Å)	13.8945(7)	13.2611(6)	15.5398(8)
<i>c</i> (Å)	12.3884(6)	16.2082(6)	16.5005(9)
<i>α</i> (deg)	90.00	100.689(2)	72.971(3)
<i>β</i> (deg)	106.686(2)	102.137(2)	76.079(3)
<i>γ</i> (deg)	90.00	109.316(2)	69.182(3)
<i>V</i> (Å ³)	2135.64(18)	2580.86(19)	3251.9(3)
<i>D_c</i> (g cm ⁻³)	1.159	1.206	1.180
<i>Z</i>	4	2	2
<i>μ</i> (mm ⁻¹)	0.068	0.269	0.228
<i>T</i> (K)	100(2)	100(2)	100(2)
<i>R_i</i> (%)	5.65	6.99	5.34
GOF	1.030	1.019	1.268

complex	7	8
formula	C ₆₇ H ₇₂ CrO ₃	C ₁₁₂ H ₁₂₄ O ₁₂ Cr ₂ ×6C ₄ H ₈ O
fw	977.28	2140.71
crystal system	monoclinic	triclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1
<i>a</i> (Å)	11.9901(5)	13.8974(15)
<i>b</i> (Å)	13.5092(5)	16.8586(18)
<i>c</i> (Å)	32.9625(14)	28.648(4)
<i>α</i> (deg)	90.00	78.612(6)
<i>β</i> (deg)	94.836(2)	85.689(6)
<i>γ</i> (deg)	90.00	76.473(5)
<i>V</i> (Å ³)	5320.1(4)	6394.3(12)
<i>D_c</i> (g cm ⁻³)	1.220	1.279
<i>Z</i>	4	4
<i>μ</i> (mm ⁻¹)	0.263	0.243
<i>T</i> (K)	100(2)	100(2)
<i>R_i</i> (%)	4.75	15.50
GOF	1.105	1.085

2. X-ray structure of HOR'

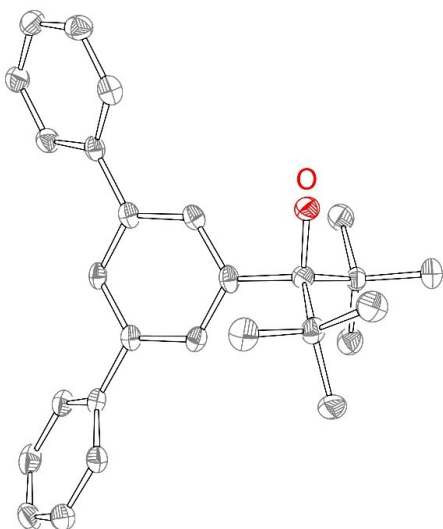


Figure S1. X-ray structure of HOR', 50% probability ellipsoids. H-atoms were omitted for clarity.

3. Evans method formula and procedure

The Evans method measurements were performed on all complexes in C₆D₆ (and in C₇D₈ for compound **2**) using a Wilmad coaxial insert (purchased from Aldrich) and a standard NMR tube. The sample was carefully weighed, and a precise amount of the appropriate NMR solvent was added to afford solutions as tabulated below. The solutions were added to the insert, and the insert was placed inside the outer NMR tube, which contained blank NMR solvent. NMR spectra were taken as indicated previously. Selected spectra are shown below (Figures S2-S4). The molar susceptibility χ_m of the compound was first calculated using Equation 1:¹

$$\chi_m = \left[\frac{3\Delta\nu}{4\pi m\nu_0} + \chi_0 \right] M \quad (1)$$

where $\Delta\nu$ is the peak separation in Hertz, m is the concentration of the solution in grams per milliliter, ν_0 is the spectrometer operating frequency in Hertz, χ_0 is the molar susceptibility of the solvent (in cm³/g), and M is the molar mass of the compound (g/mol).

χ_d was then calculated using Pascal constants, and was applied to correct the value of χ_m for the diamagnetic susceptibility to give the value of χ_p .

The solution state effective magnetic moment (μ_{eff}) was calculated using Equation 2:

$$\mu_{eff} = \sqrt{(2.383 \times 10^3)(\chi_p)} \quad (2)$$

Several measurements were taken for each compound, and the average of them was taken. We estimate experimental error to be at least 10-15% of the value attributed to the error in mass and volume.

Table S2. Magnetic moments for complexes **2-7** using the Evans method.

Complex 2 (Benzene)	Solvent	μ_{obs} (μ_B)
4	C ₆ D ₆	4.23
5	C ₆ D ₆	4.23
6	C ₆ D ₆	4.20
average	---	4.2
estimated error	---	0.5

Complex 2 (Toluene)	Solvent	μ_{obs} (μ_B)
1	C ₇ D ₈	4.25
2	C ₇ D ₈	4.15
3	C ₇ D ₈	4.03
average	---	4.2
standard deviation	---	0.5

Complex 3	$\mu_{\text{obs}} (\mu_{\text{B}})$
1	2.20
2	2.38
3	2.62
average	2.4
estimated error	0.3

Complex 4	$\mu_{\text{obs}} (\mu_{\text{B}})$
1	2.45
2	2.21
3	2.30
average	2.3
estimated error	0.3

Complex 5	$\mu_{\text{obs}} (\mu_{\text{B}})$
1	2.82
2	2.31
3	2.35
average	2.5
estimated error	0.3

Complex 6	$\mu_{\text{obs}} (\mu_{\text{B}})$
1	2.60
2	2.40
3	2.70
average	2.6
estimated error	0.3

Complex 7	$\mu_{\text{obs}} (\mu_{\text{B}})$
1	3.81
2	4.03
3	3.50
average	3.8
estimated error	0.4

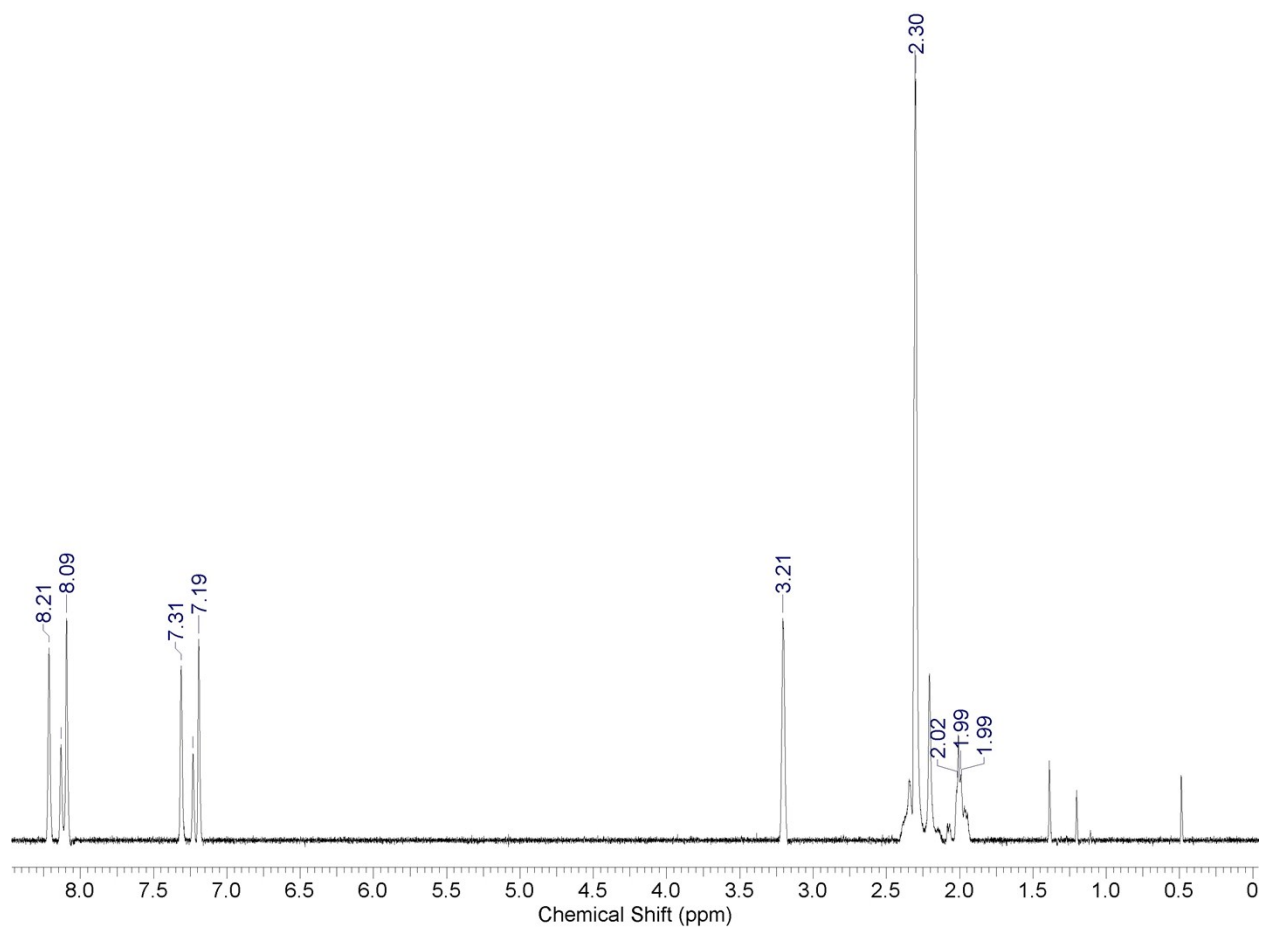


Figure S2. ^1H NMR of $\text{Cr}(\text{OR}')_2(\text{THF})_2$ using the Evans method in C_7D_8 ($4.25 \mu\text{B}$).

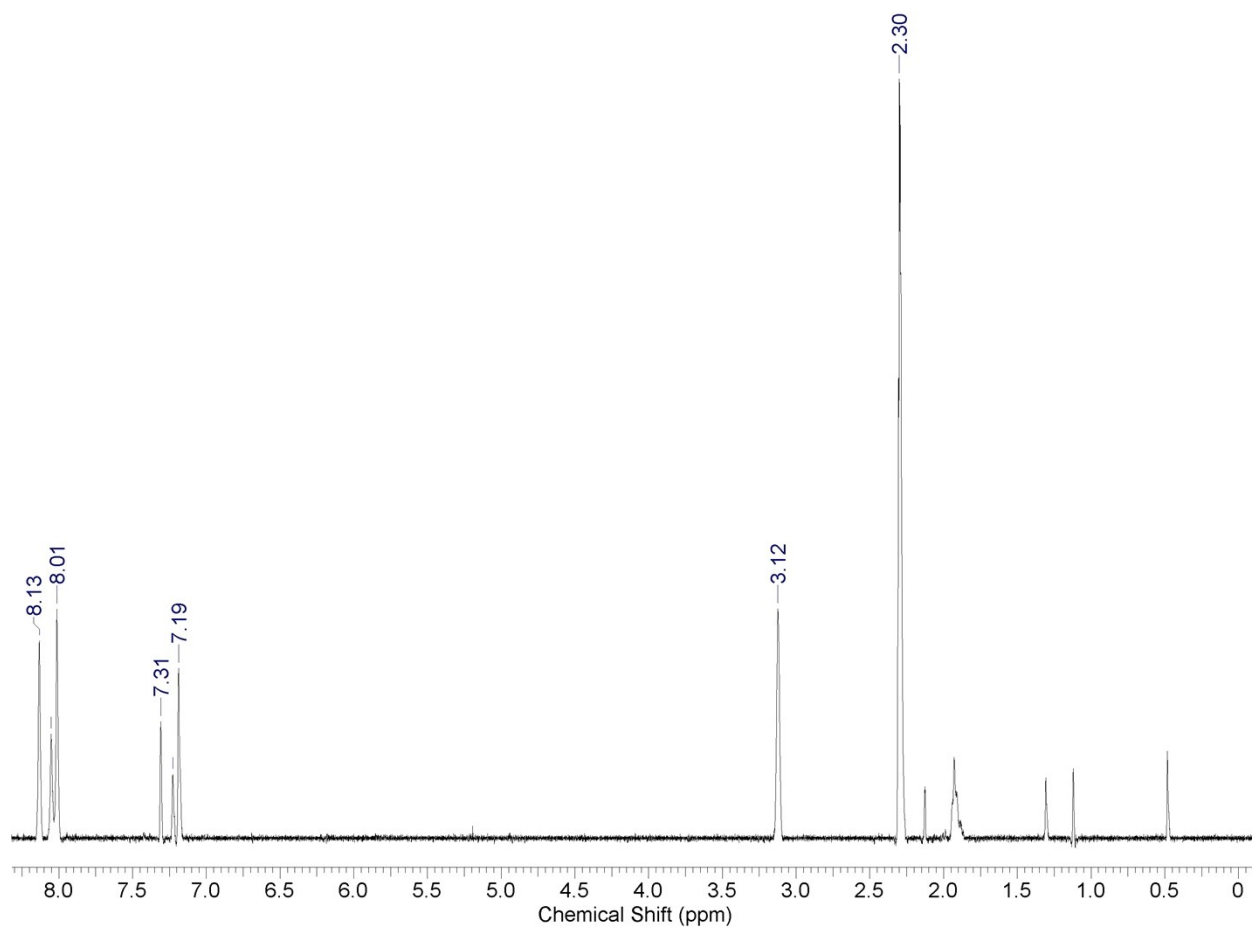


Figure S3. ^1H NMR of $\text{Cr}(\text{OR}')_2(\text{THF})_2$ using the Evans method in C_7D_8 ($4.03\mu\text{B}$).

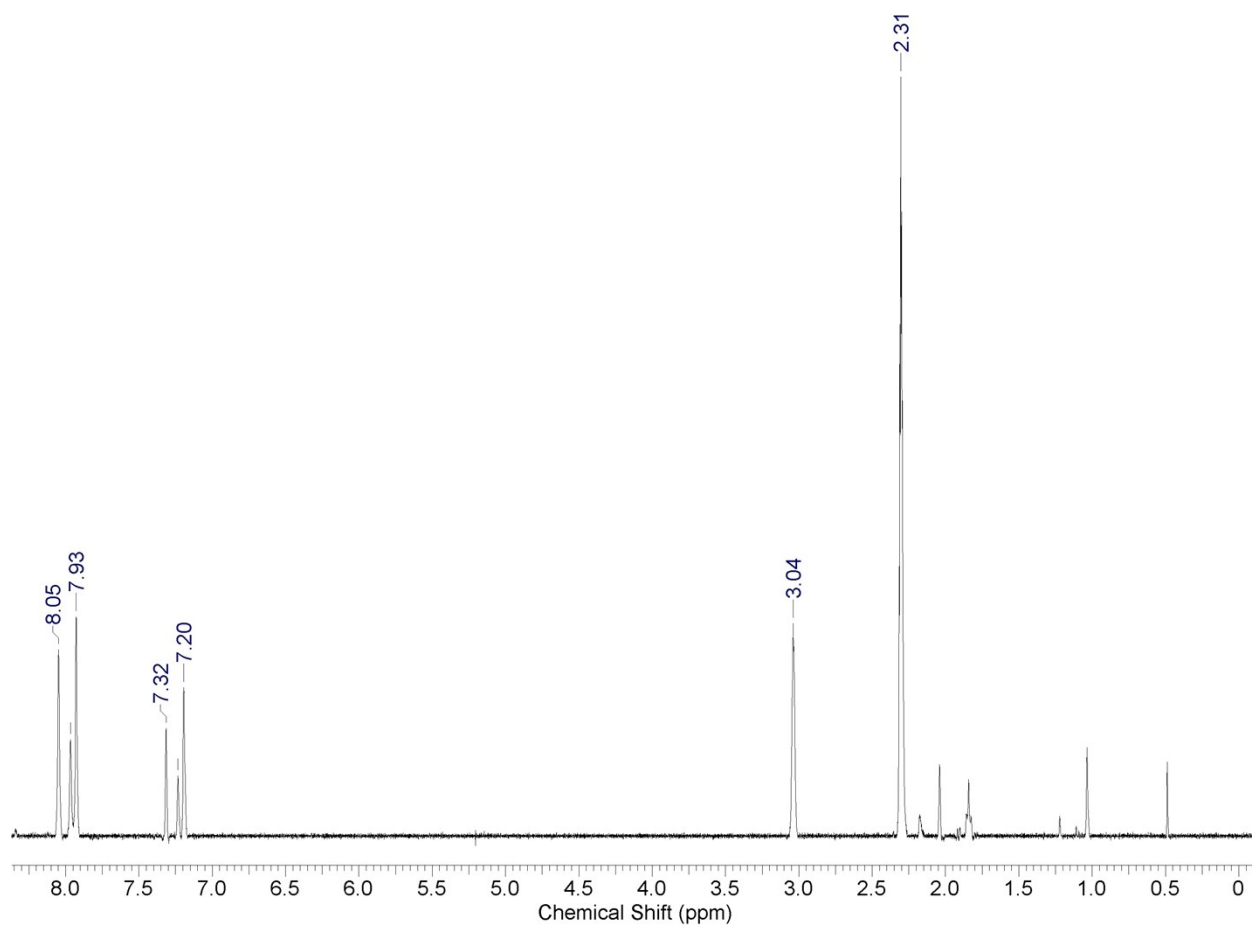


Figure S4. ^1H NMR of $\text{Cr}(\text{OR}')_2(\text{THF})_2$ using the Evans method in C_7D_8 ($4.15\mu\text{B}$).

4. NMR Spectra

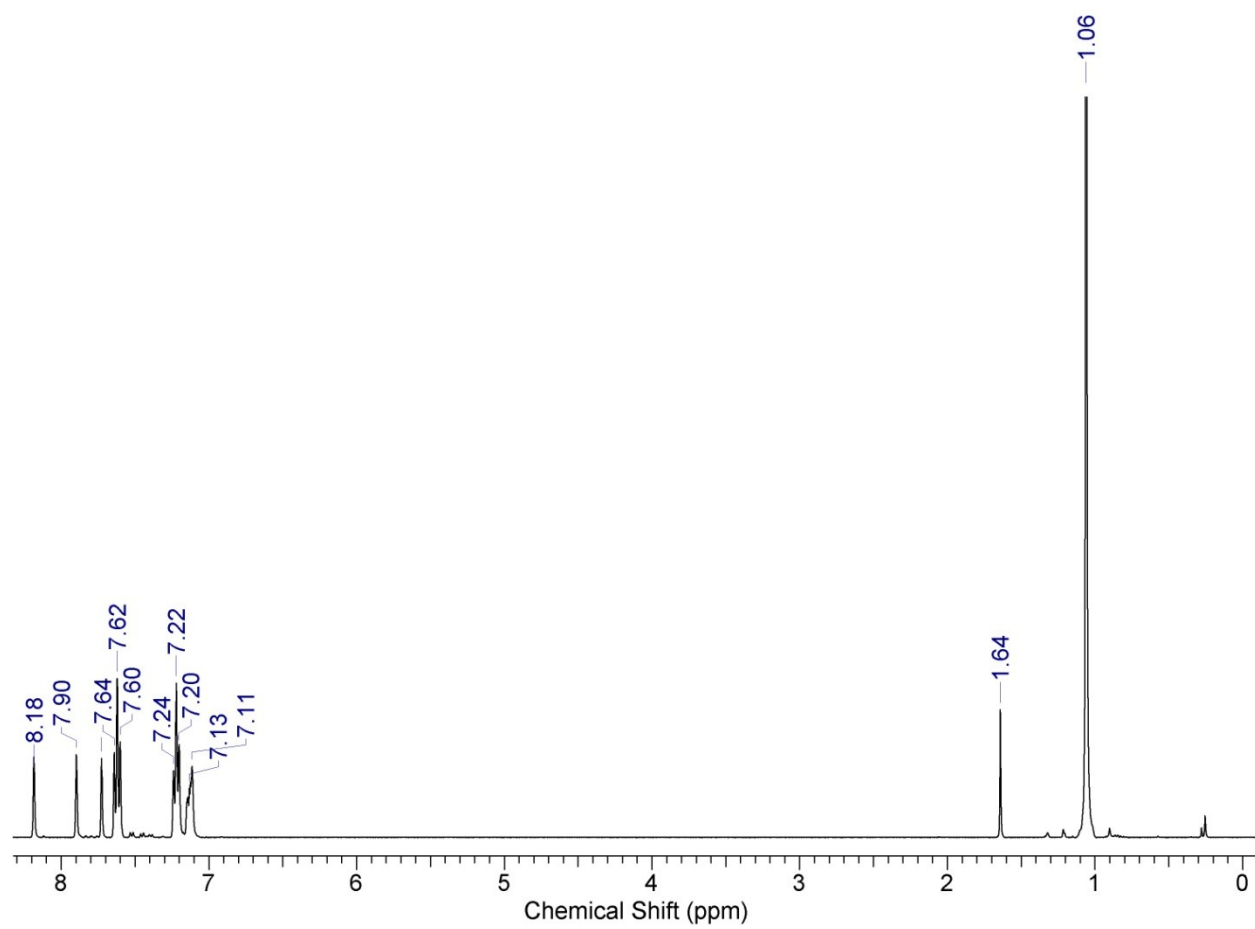


Figure S5. ^1H NMR of HOR' in C_6D_6 .

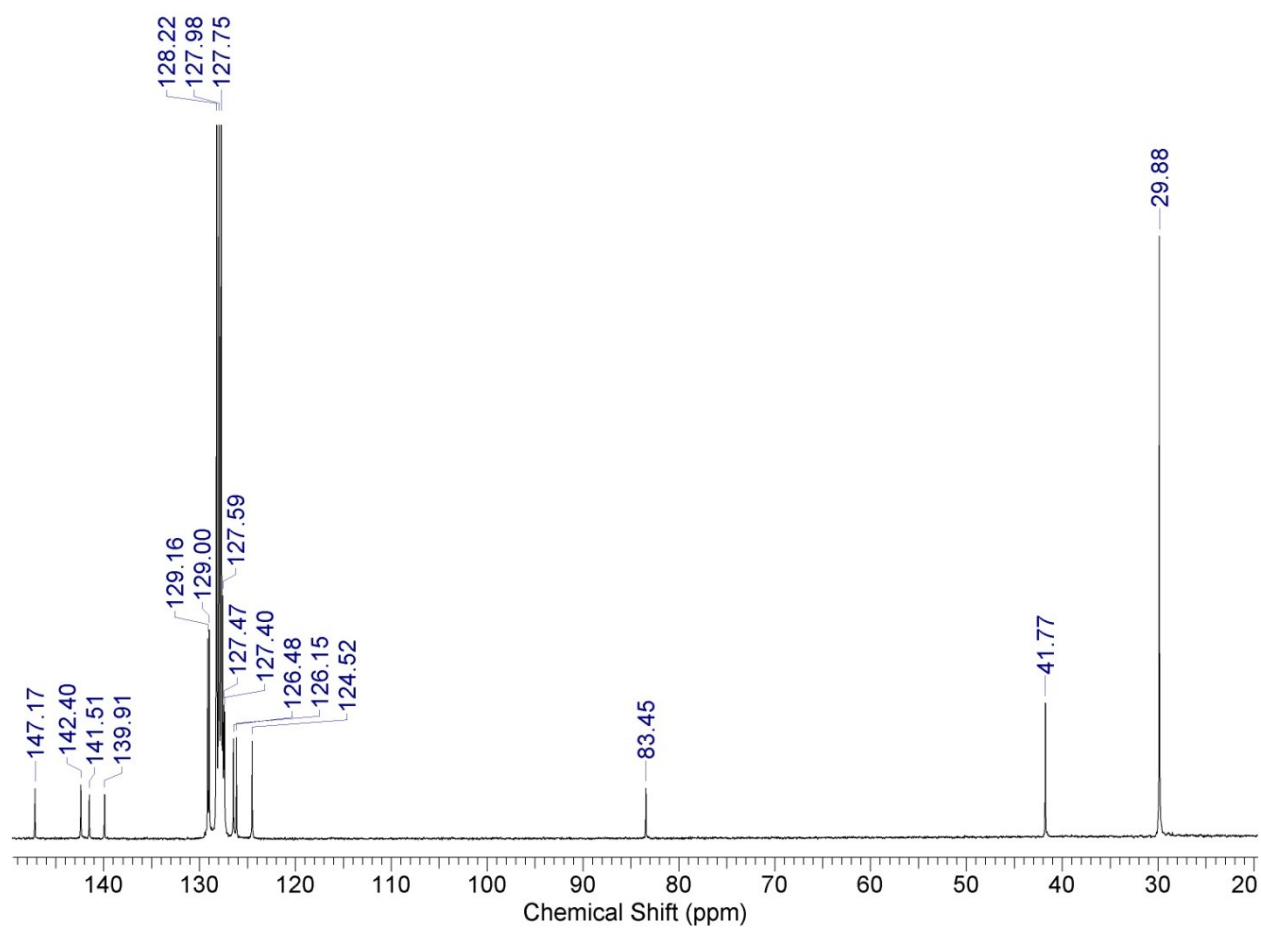


Figure S6. ¹³C NMR of HOR' in C₆D₆.

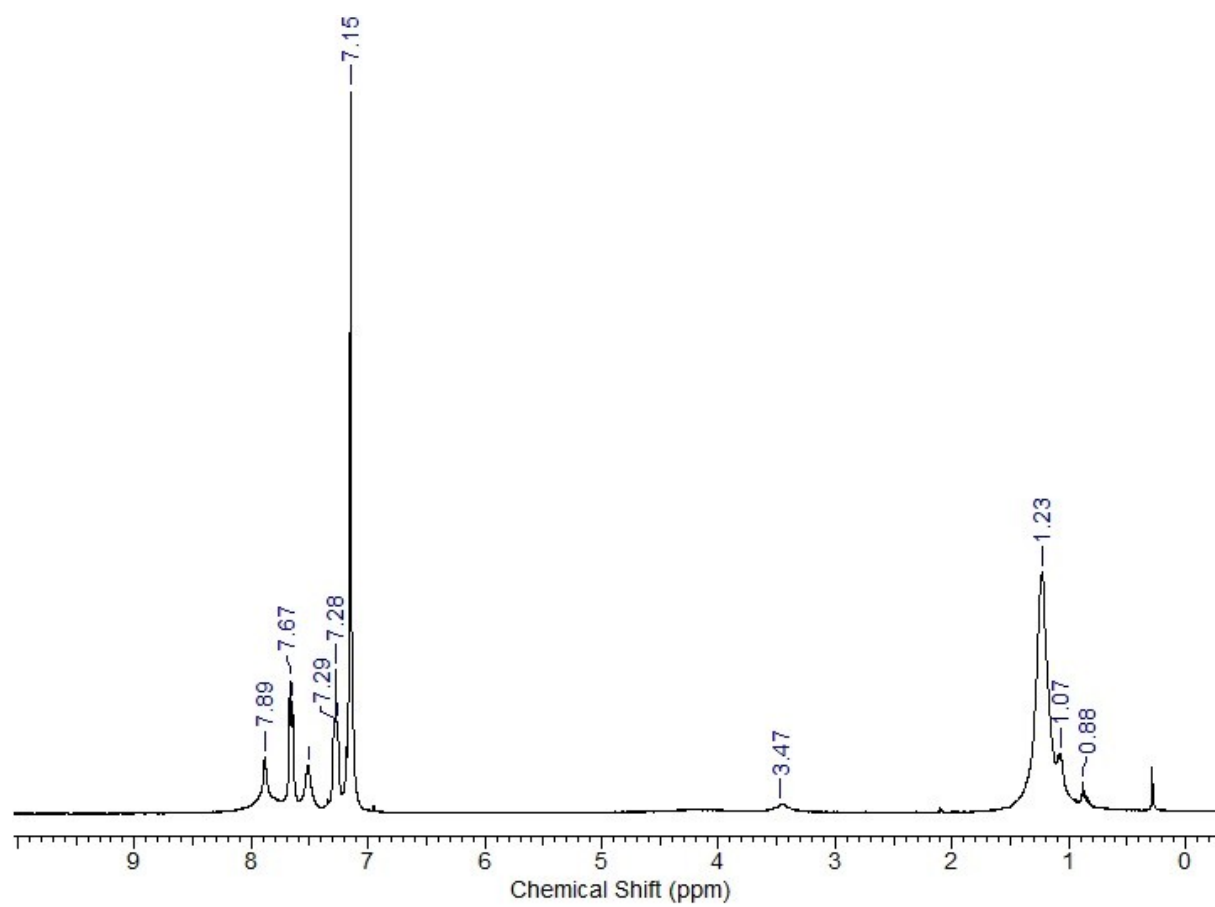


Figure S7. ^1H NMR of complex **8** $\text{Cr}_2(\text{O}_2\text{COR}')_4(\text{THF})_2$ in C_6D_6 .

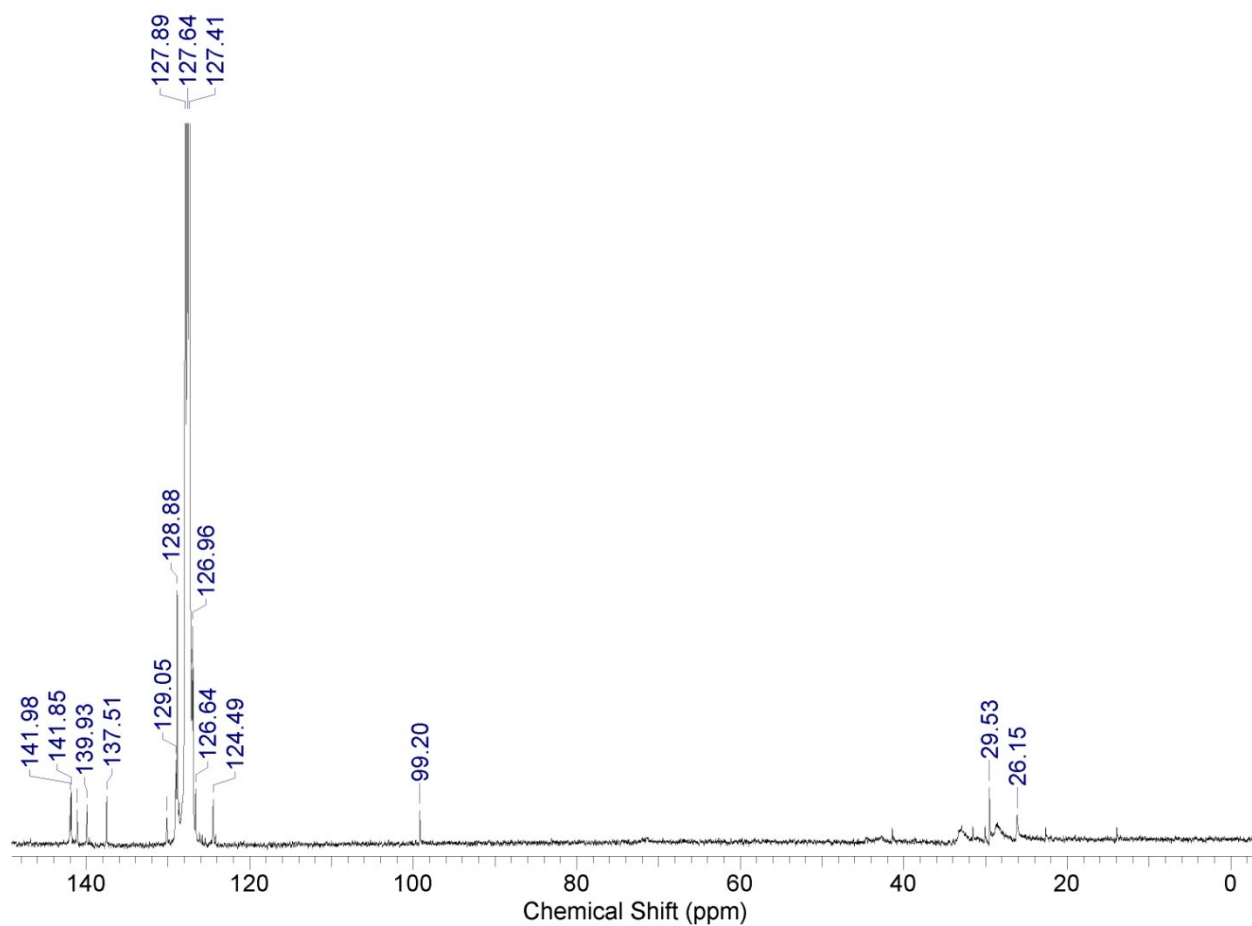


Figure S8. ^{13}C NMR of complex **8** $\text{Cr}_2(\text{O}_2\text{COR}')_4(\text{THF})_2$ in C_6D_6 .

5. IR Spectra

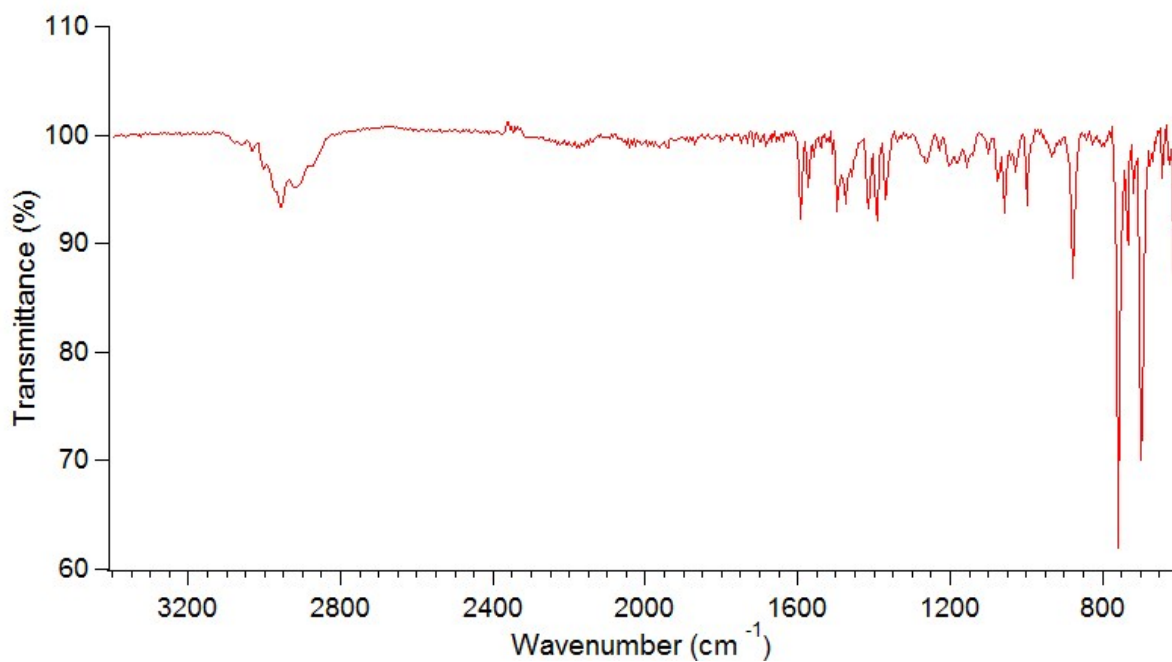


Figure S9. IR spectra of complex HOR' in the 3400-600 cm⁻¹ range.

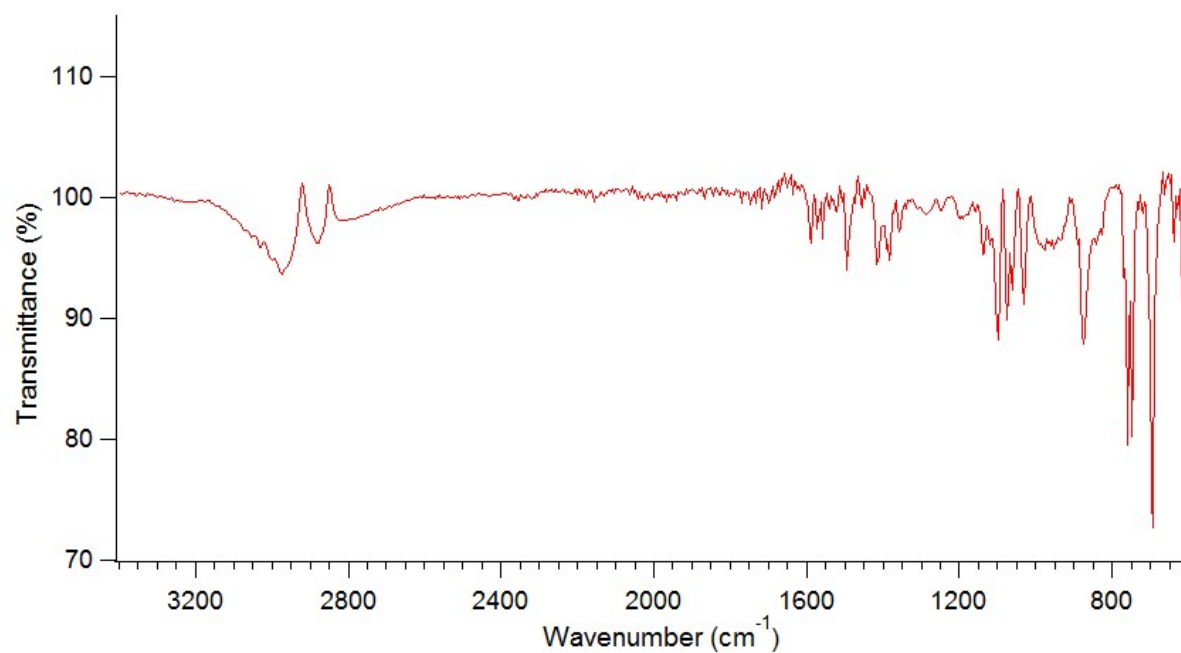


Figure S10. IR spectra of complex **2** $\text{Cr}(\text{OR}')_2(\text{THF})_2$ in the 3400-600 cm^{-1} range.

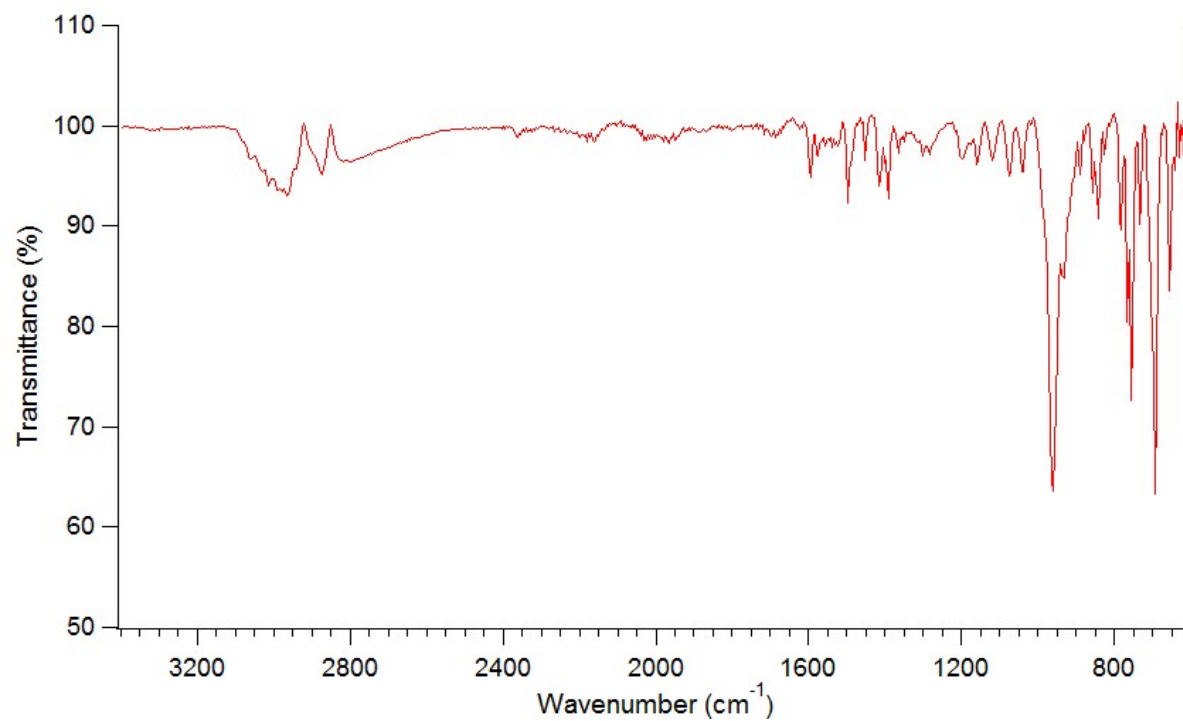


Figure S11. IR spectra of complex **3** in the 3400-600 cm^{-1} range.

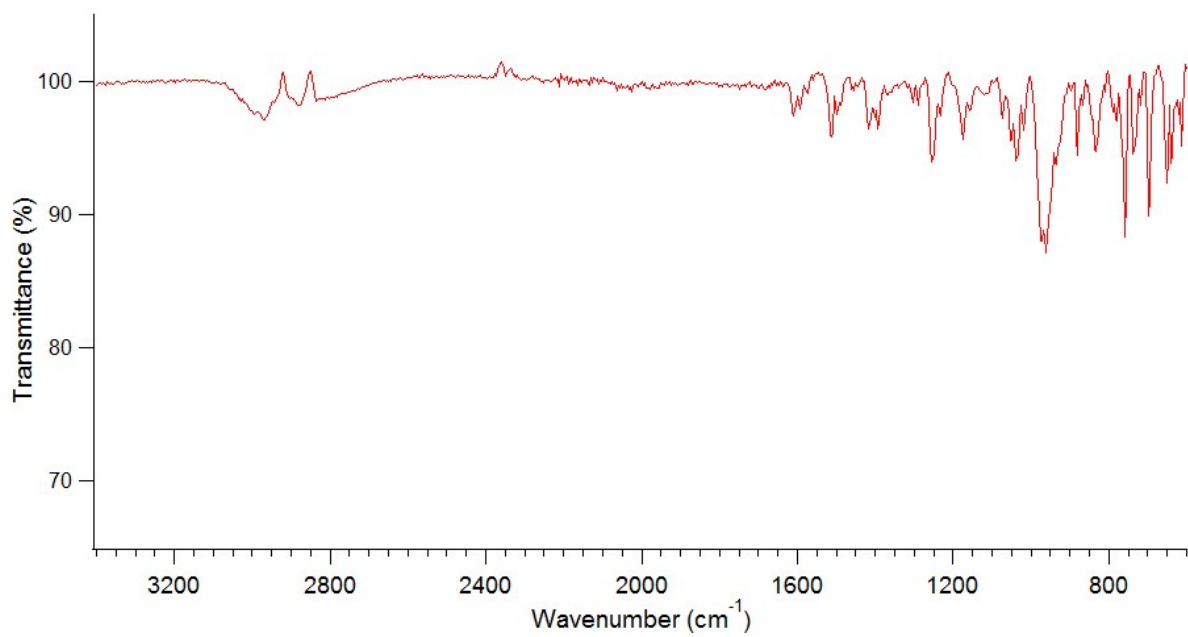


Figure S12. IR spectra of complex **4** in the 3400-600 cm^{-1} range.

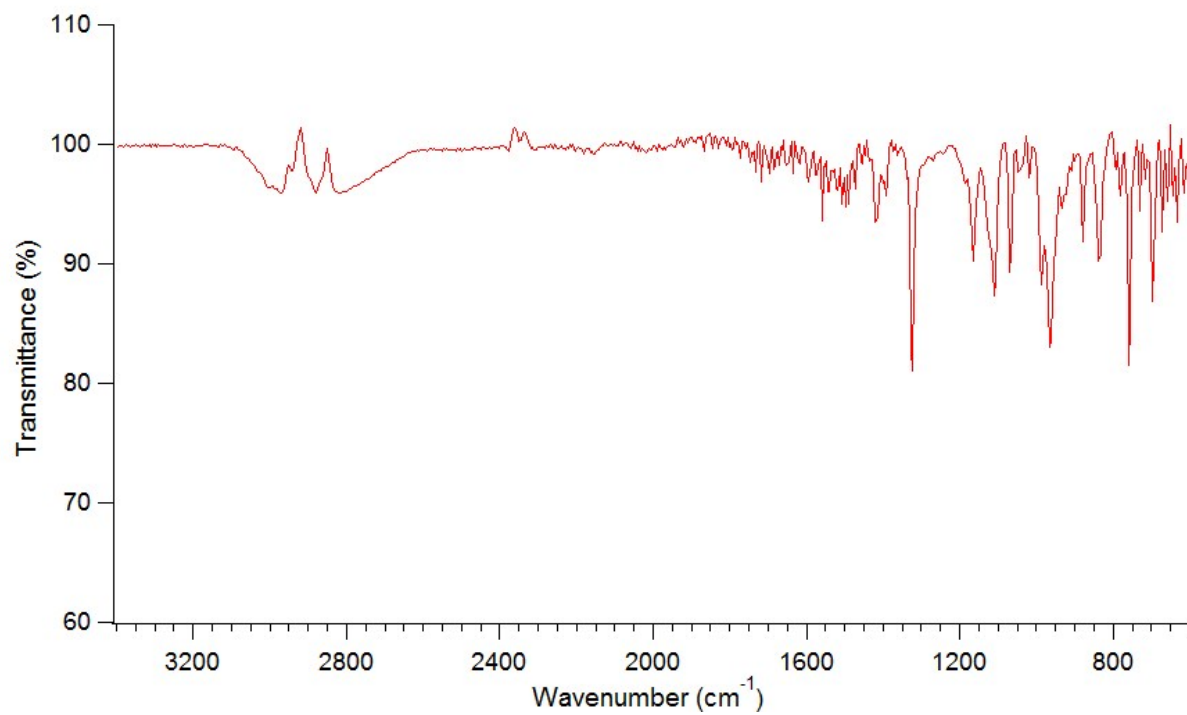


Figure S13. IR spectra of complex **5** in the 3400-600 cm^{-1} range.

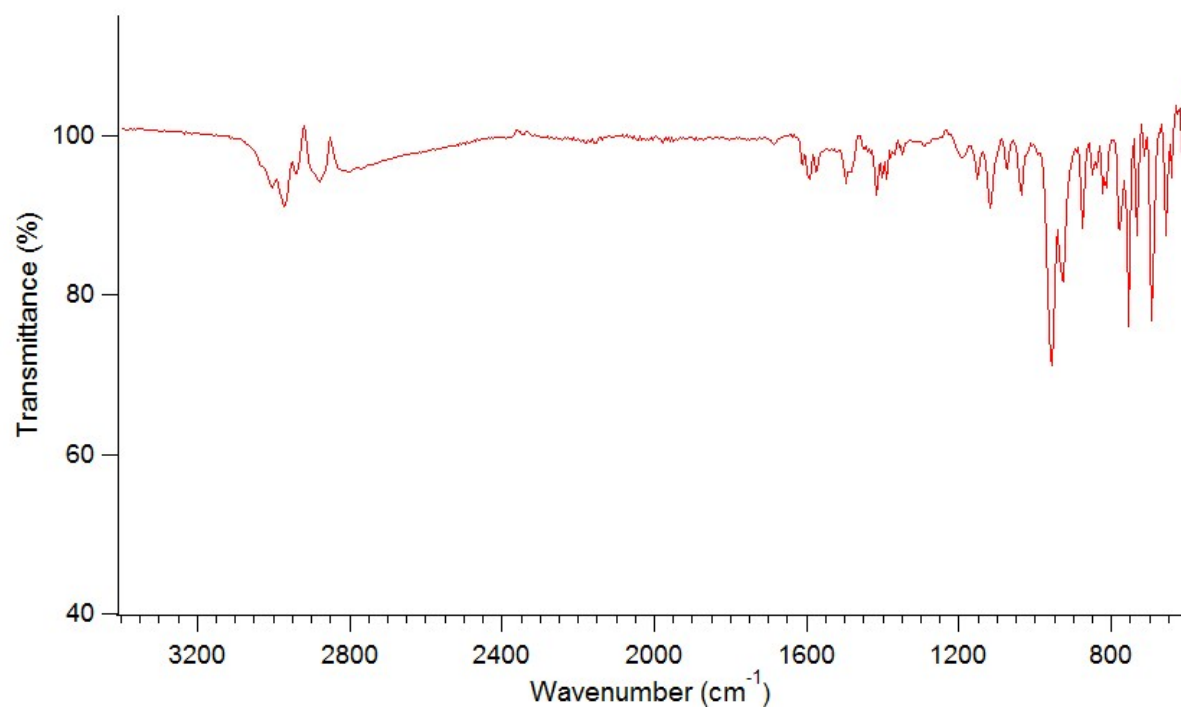


Figure S14. IR spectra of complex **6** in the 3400-600 cm^{-1} range.

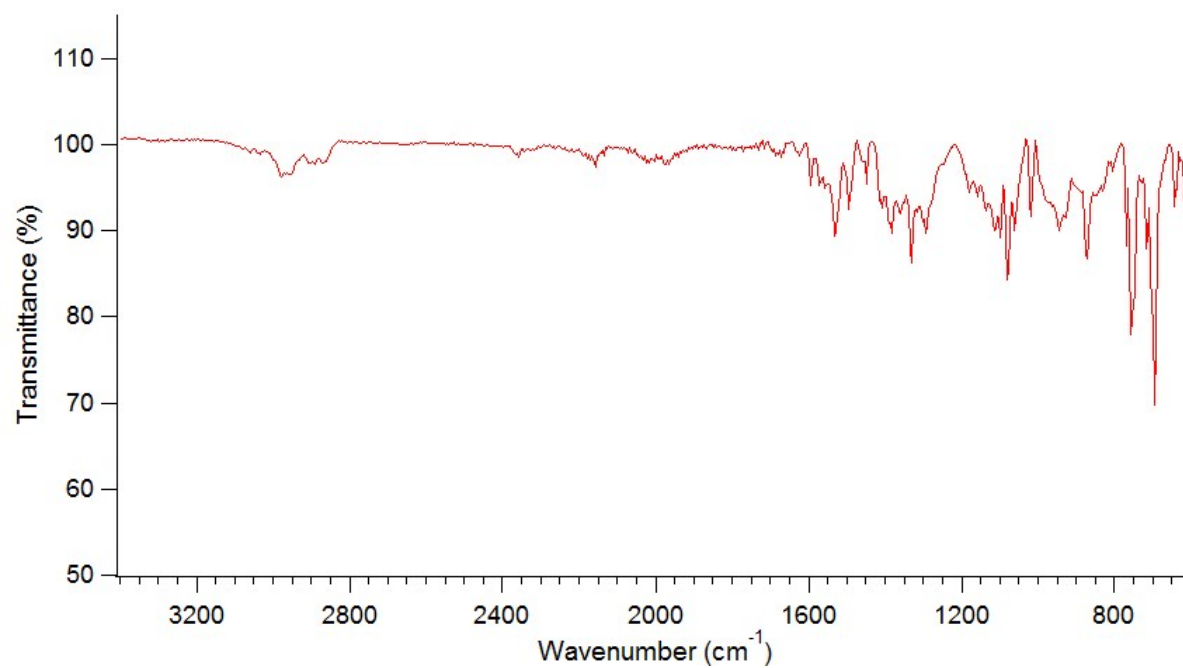


Figure S15. IR spectra of complex **7** in the 3400-600 cm^{-1} range.

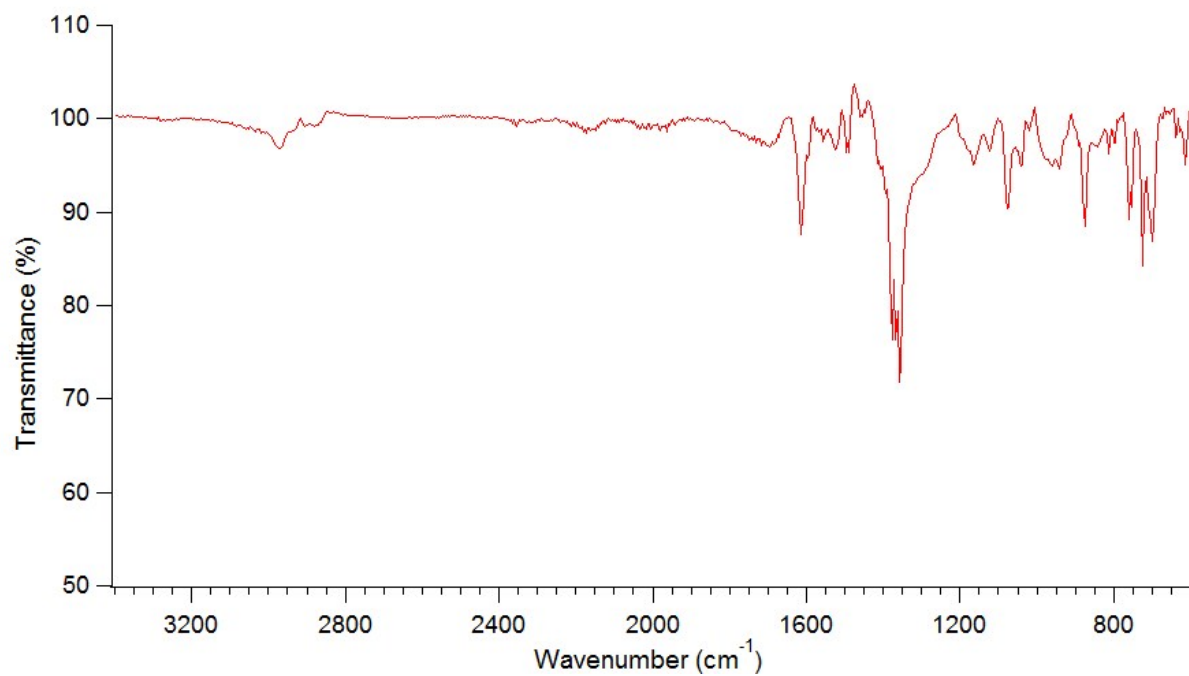


Figure S16. IR spectra of complex **8** in the 3400-600 cm^{-1} range.

6. UV-vis spectra

The UV-vis spectra of the Cr(IV)-diolate complexes **3-5** are presented in **Figure S14** and are compared to the corresponding spectrum of complex **7**. **Figure S14** demonstrates that the spectra of compounds **3-5** (taken in THF) display very similar spectra featuring single band in the visible region at 615 ± 5 nm. In contrast, complex **7** has a single broad peak centered at 710 nm. We note that complex **6** (whose spectrum taken in a toluene due to its instability in THF, **Figure S19**) demonstrates an additional spectral feature (shoulder) around 690 ppm, in addition to the expected peak at 611 nm.

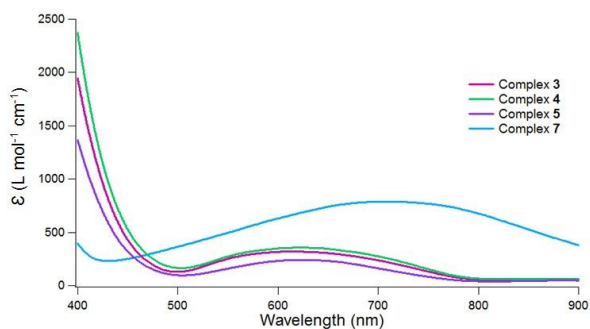


Figure S17. The absorption spectra of complexes **3 - 5** and **7** in 400 – 900 nm region.

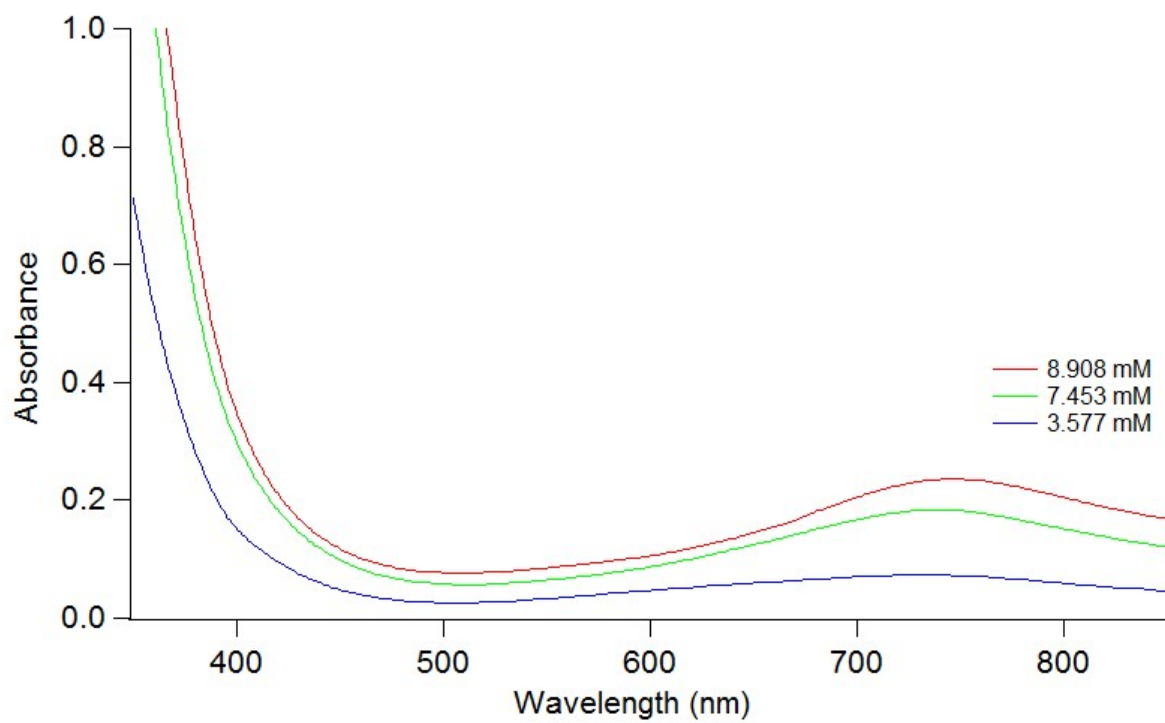


Figure S18. UV-vis spectrum for complex **2** $\text{Cr}(\text{OR}')_2(\text{THF})_2$ at three different concentrations. λ_{max} (ϵ_M): 730 (24).

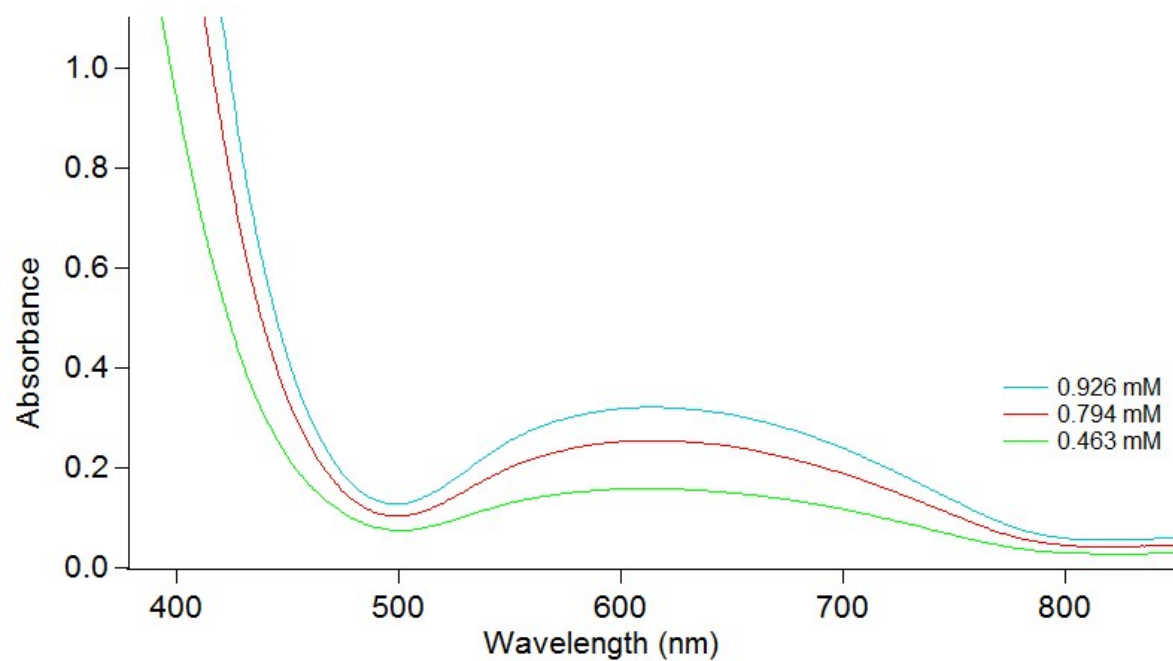


Figure S19. UV-vis spectrum for complex **3** $\text{Cr}(\text{OR}')_2(\text{O}_2\text{C}_2\text{H}_2\text{Ph}_2)$ at three different concentrations. λ_{max} (ϵ_{M}): 614 (336).

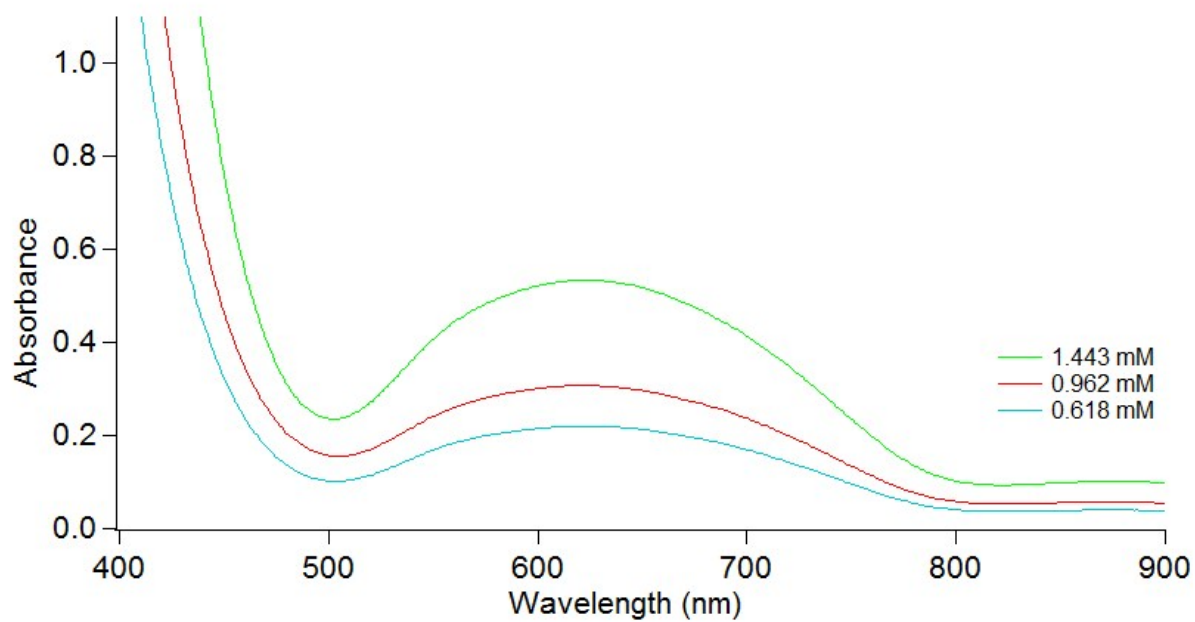


Figure S20. UV-vis spectrum for complex **4** $\text{Cr}(\text{OR}')_2(\text{O}_2\text{C}_2\text{H}_2(4\text{-CH}_3\text{OPh})_2)$ at three different concentrations. λ_{max} (ϵ_{M}): 624 (350).

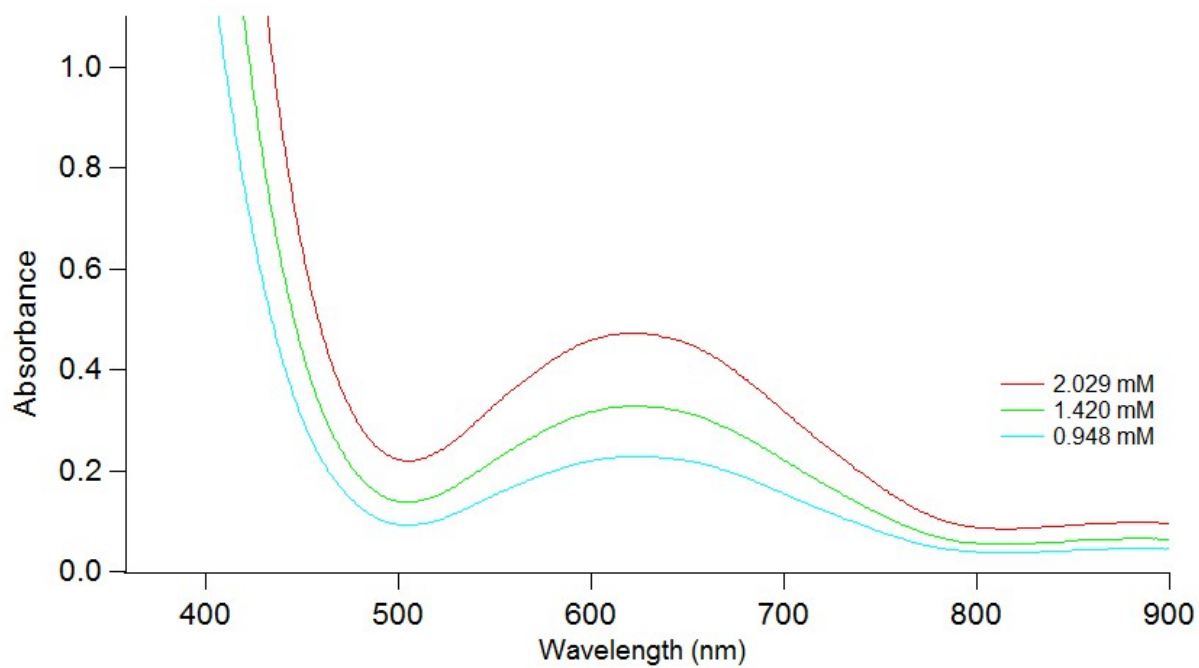


Figure S21. UV-vis spectrum for complex **5** $\text{Cr}(\text{OR}')_2(\text{O}_2\text{C}_2\text{H}_2(4\text{-F}_3\text{CPh})_2)$ at three different concentrations. λ_{max} (ϵ_{M}): 620 (235).

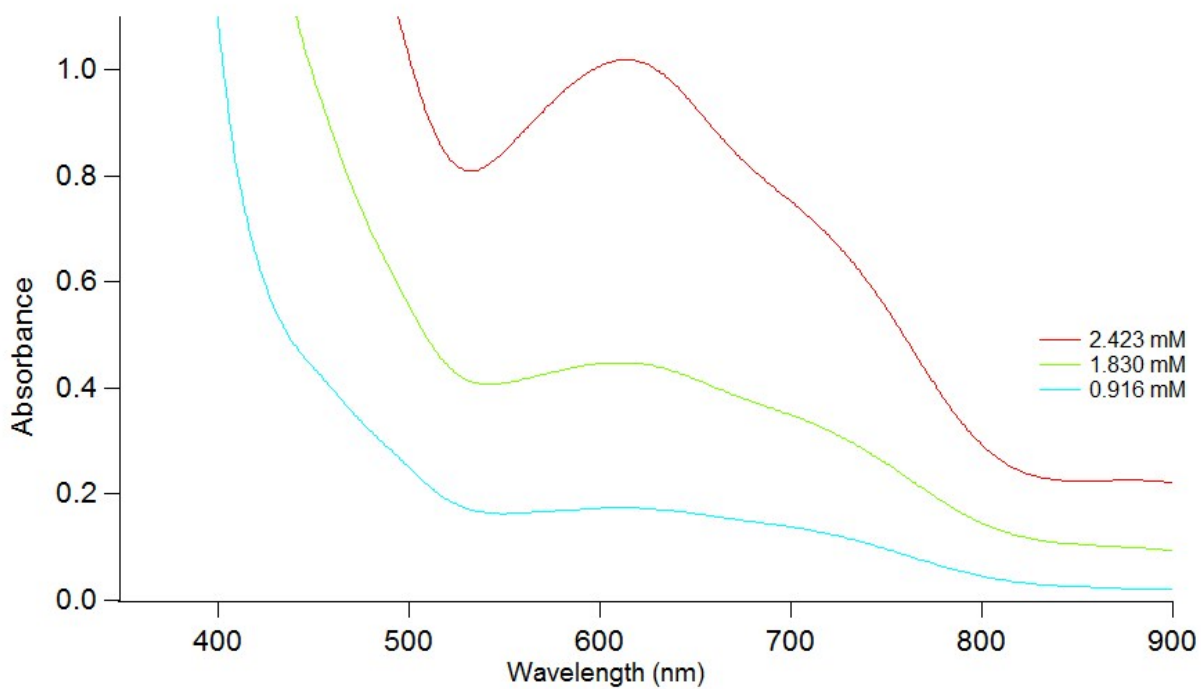


Figure S22. UV-vis spectrum for complex **6** $\text{Cr}(\text{OR}')_2(\text{O}_2\text{C}_2\text{H}_2(2,4,6\text{-Me}_3\text{Ph})_2)$ at three different concentrations. λ_{max} (ϵ_{M}): 611 (234).

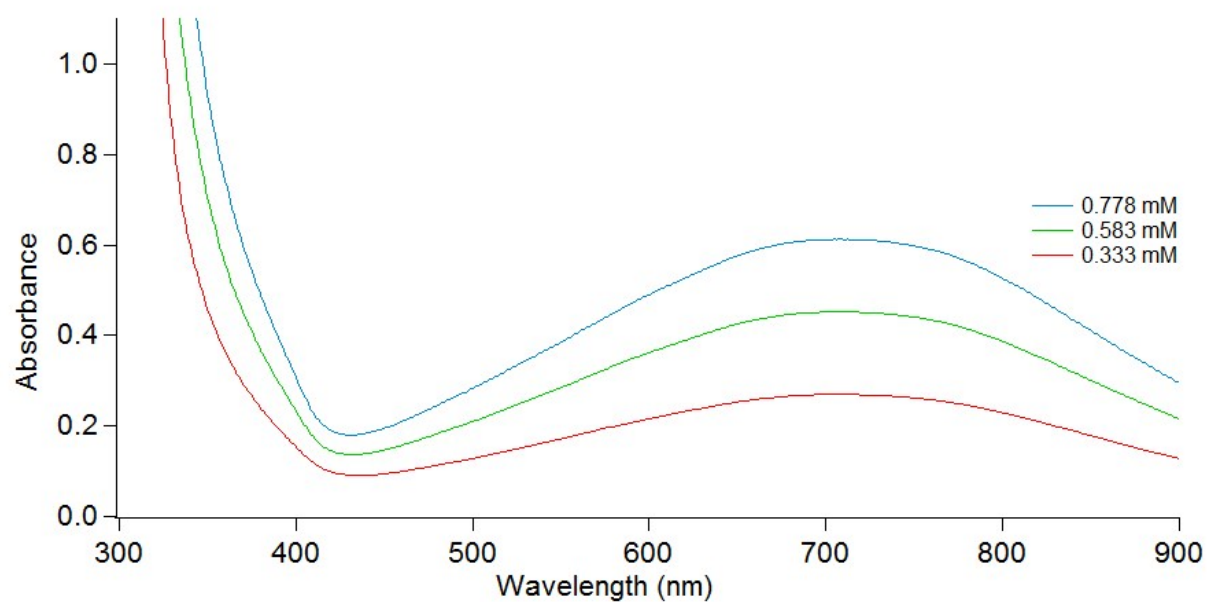


Figure S23. UV-vis spectrum for complex **7** $\text{Cr}(\text{OR}')_2(\text{OCPh}_2)$ at three different concentrations. λ_{max} (ϵ_M): 707 (800).

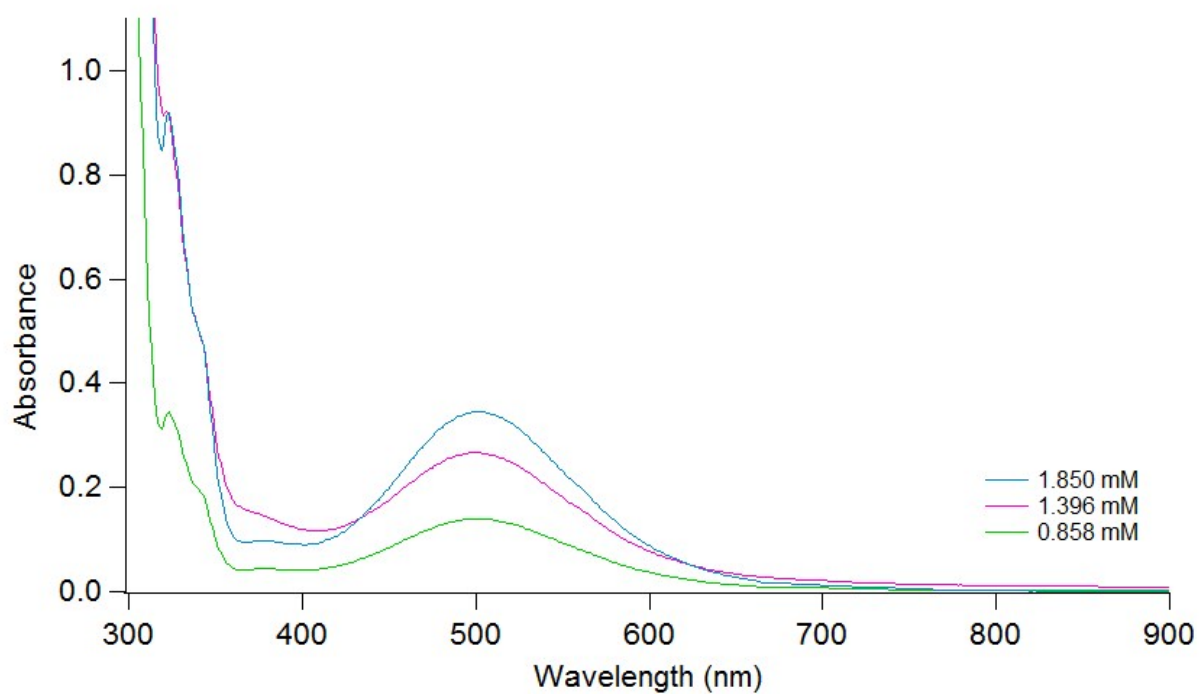


Figure S24. UV-vis spectrum for complex **8** $\text{Cr}_2(\text{O}_2\text{COR})_4(\text{THF})_2$ at three different concentrations. λ_{max} (ϵ_M): 502 (223).

7. Computational results

Full reference for Gaussian 09: Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

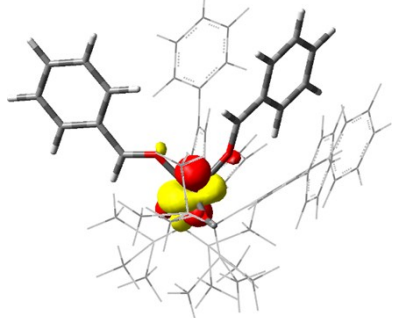
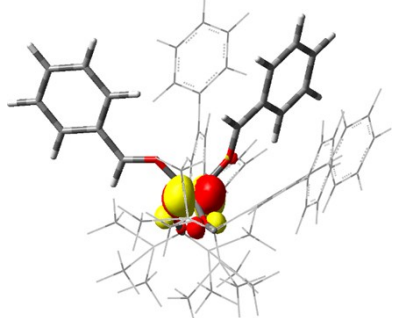
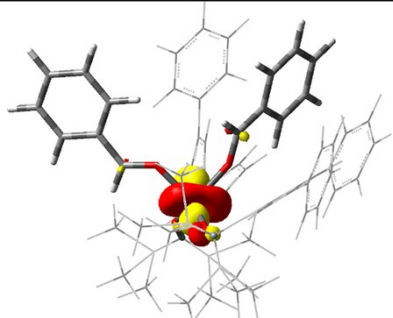
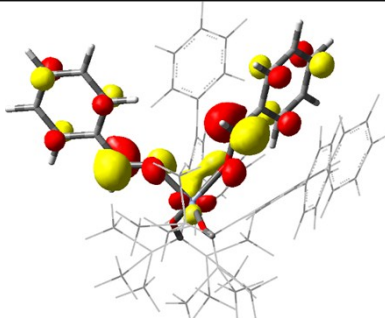
alpha	overlap	beta
	—	—
	—	—
	0.47	

Figure S25. Corresponding orbital isosurface plots (iso = 0.05 au) for triplet **3**.

Table S3. Cartesian coordinates (Å) for each optimized structure.

----				C	-3.91797100	-3.39431900	0.17662500
bis-benzaldehyde singlet				H	-3.32312700	-2.99140500	1.02096000
----				H	-4.85160200	-2.79981600	0.09668300
Cr	0.25115200	-1.13760600	0.01691400	H	-4.22985700	-4.42783900	0.44322100
O	1.64120000	-1.82056800	-0.87230800	C	-4.06647600	-3.83919200	-2.26579400
O	-1.27462200	-1.95381500	-0.46758700	H	-4.50766400	-4.82328600	-1.99350900
C	3.06924400	-2.04933000	-0.79972500	H	-4.92953300	-3.17124200	-2.41197400
C	-2.42245200	-1.90040900	-1.34816100	H	-3.54670100	-4.01193500	-3.22500900
O	-0.09335500	-1.50633000	1.88672700	C	-0.93823300	-2.57093400	-3.39642600
O	0.50833500	0.56912800	0.49290900	H	-0.38269200	-2.17792300	-4.27559700
C	0.83702000	1.65562000	1.06472600	H	-0.19130700	-2.89132100	-2.64430300
H	1.72388900	1.63660900	1.70488700	H	-1.49370700	-3.44981800	-3.77088600
C	-0.73613000	-2.40049300	2.48448600	C	-2.96462800	-1.18510700	-3.88166800
H	-1.18288800	-3.21382500	1.90510800	H	-2.49070000	-1.04951200	-4.87863400
C	0.14467800	2.90403900	0.87552900	H	-3.71520900	-1.97780800	-4.00756700
C	-0.86777600	3.05860500	-0.09536500	H	-3.48684600	-0.22806300	-0.26729200
C	0.50522500	4.02349000	1.65675200	C	-1.04242100	-0.19332000	-2.70127500
C	-1.49268000	4.28562100	-0.27470100	H	-0.64146400	0.11418900	-3.69219100
H	-1.13700200	2.20799300	-0.70850600	H	-1.66005300	0.64776200	-2.32746000
C	-0.13060700	5.24623400	1.47788300	H	-0.17599200	-0.32024000	-0.203117500
H	1.28836500	3.91997600	2.40443600	C	3.75285800	-0.65363800	-0.82953000
C	-1.13154200	5.38629200	0.51055500	C	5.12407000	-0.47056700	-0.55331000
H	-2.26561700	4.38831900	-1.03177300	C	3.01698200	0.49167200	-1.21202700
H	0.15575700	6.09703000	2.09036900	C	5.72088200	0.80065000	-0.57632400
H	-1.62325900	6.34426600	0.36807100	H	5.75074400	-1.30772700	-0.33205000
C	-0.91043600	-2.40398000	3.92231500	C	3.59038700	1.77235400	-1.23614900
C	-1.65808700	-3.43412500	4.52329400	H	1.98745500	0.39738200	-1.51210100
C	-0.36031800	-1.38729100	4.72938000	C	4.94240300	1.91802000	-0.90313800
C	-1.85414300	-3.44731500	5.90075400	H	5.40496500	2.89624000	-0.95271000
H	-2.08484600	-4.21654600	3.89991900	C	-3.34755400	-0.77453800	-0.80432800
C	-0.55838700	-1.40687600	6.10342600	C	-4.63410500	-0.53252000	-1.33186100
H	0.20599000	-0.59321900	4.25344500	C	-2.93665600	0.03209200	0.28363300
C	-1.30512900	-2.43497700	6.69331000	C	-5.48137700	0.45091000	-0.79592600
H	-2.43403600	-4.24363900	6.35881600	H	-4.99246700	-1.08738000	-2.17552800
H	-0.13632500	-0.61978100	6.72227900	C	-3.76956800	1.01673200	0.83858500
H	-1.45977600	-2.44440700	7.76875100	C	-1.95433900	-0.08138500	0.70594500
C	3.27415100	-2.82595700	0.61359600	C	-5.04251200	1.21710500	0.29116500
C	3.44159800	-2.82093200	-2.15769800	H	-5.70839000	1.94824100	0.73281000
C	2.90865800	-2.01014500	-3.37833700	C	-3.30173600	1.83605400	1.98985200
H	1.82103900	-1.82323500	-3.30849900	C	-2.52107700	1.25932900	3.01098300
H	3.41682600	-1.02752600	-3.46995500	C	-3.60716100	3.20870700	2.06461600
H	3.09184600	-2.55115600	-4.33246300	C	-2.04122200	2.04118400	4.06537500
C	4.96379100	-2.99451200	-2.42206200	H	-2.29092100	0.20251400	3.00082700
H	5.50827700	-3.48411200	-1.60266700	C	-3.12592100	3.98563200	3.12259100
H	5.12634500	-3.62275200	-3.32511800	H	-4.18646500	3.69062000	1.28704300
H	5.45715000	-2.02423300	-2.63525900	C	-2.34015900	3.40375500	4.11923900
C	2.77820600	-4.21677900	-2.24194200	H	-1.43834600	1.58944100	4.84244200
H	2.82263600	-4.61915300	-3.27739700	H	-3.35180400	5.04334600	3.16207000
H	3.30671500	-4.96012600	-1.61736400	H	-1.96372400	4.00870900	4.93381000
H	1.70822400	-4.17438900	-1.95312300	C	-6.83354800	0.67028400	-1.36907300
C	4.57781500	-3.64792900	0.79385700	C	-7.32672000	1.97512200	-1.55767400
H	4.62934200	-4.50973000	0.10396400	C	-7.64247200	-0.42309300	-1.73287400
H	5.50139100	-3.05662800	0.72524000	C	-8.59943900	2.17913800	-2.09945100
H	4.60327300	-4.09224600	1.81344600	H	-6.72176000	2.83614100	-1.30195000
C	2.12100800	-3.84531000	0.89503200	C	-8.91459900	-0.21308100	-2.27358100
H	2.20337000	-4.76231100	0.28556200	H	-7.29808300	-1.43899100	-1.58361700
H	2.14717800	-4.19639400	1.94982300	C	-9.39252700	1.08643400	-2.45703400
H	1.11399200	-3.42616800	0.73039100	H	-8.96968100	3.18572700	-2.24510800
C	3.23178300	-1.79522200	1.77776900	H	-9.53168400	-1.05908500	-2.54744200
H	4.16122700	-1.19142500	1.82072900	H	-10.37752700	1.24669000	-2.87601800
H	2.37912800	-1.09843600	1.66190100	C	2.77393000	2.96638300	-1.61464200
H	3.13769300	-2.29220300	2.76777000	C	1.82801400	2.87530500	-2.65561500
C	-1.88116700	-1.49654500	-2.81068200	C	2.92053600	4.17481000	-0.92433600
C	-3.10225500	-3.36390200	-1.15016000	C	1.04828900	3.98549900	-2.99251500
C	-2.03698800	-4.49841500	-1.00157100	H	1.69989200	1.95964100	-3.21890800
H	-1.32765500	-4.31227900	-0.17098900	C	2.14032600	5.28263600	-1.26837500
H	-2.52608400	-5.47116900	-0.77473600	H	3.61900600	4.26363300	-0.10191800
H	-1.45722200	-4.67184400	-1.92282200	C	1.20493000	5.18807300	-2.30057200

H	0.32188800	3.91297800	-3.79152100	H	2.52834100	-4.26436900	2.10390500
H	2.25220100	6.21188700	-0.72496500	H	1.36207600	-3.44786400	1.05046600
H	0.59637300	6.04474400	-2.55940300	C	3.46837600	-1.79355900	1.86043100
C	7.16556500	0.95878000	-0.27211500	H	4.34800100	-1.11970300	1.82422600
C	7.61186400	2.01672600	0.54198800	H	2.54797300	-1.17520800	1.81417300
C	8.11047200	0.05440100	-0.79304100	H	3.49579200	-2.28619200	2.85692000
C	8.97238300	2.16334600	0.82911800	C	-1.95544100	-1.53215800	-2.83530200
H	6.90718400	2.71943600	0.96902200	C	-3.32329600	-3.35325300	-1.23377000
C	9.46978100	0.20630700	-0.50313900	C	-2.32652200	-4.54363600	-1.06357900
H	7.80044100	-0.75865600	-1.43768600	H	-1.65203200	-4.40761400	-0.19344800
C	9.90033800	1.25919700	0.30733400	H	-2.87448200	-5.49449100	-0.88307200
H	9.30696800	2.97714500	1.45943600	H	-1.71124500	-4.72402000	-1.96011600
H	10.19032400	-0.49118500	-0.91037700	C	-4.18304800	-3.35610500	0.06528300
H	10.95307100	1.37475300	0.53061700	H	-3.59308400	-3.00514800	0.93569000
----				H	-5.07643700	-2.70503200	-0.03336600
bis-benzaldehyde triplet				H	-4.56444700	-4.37355900	0.30186300
----				C	-4.27612300	-3.75589300	-2.38656100
Cr	0.18791100	-1.36441600	0.00248400	H	-4.77836800	-4.71906000	-2.14741300
O	1.75974100	-1.90507300	-0.68300400	H	-5.09547000	-3.03604900	-2.54281500
O	-1.42115200	-2.05035700	-0.51642900	H	-3.73822300	-3.93692800	-3.33382000
C	3.18723100	-2.08322500	-0.70424700	C	-1.05778500	-2.64982800	-3.41822600
C	-2.55743300	-1.92902300	-1.39294200	H	-0.46345900	-2.27271900	-4.27925400
O	-0.15058200	-1.58012400	1.89072500	H	-0.33721800	-3.01941400	-2.65953700
O	0.20450700	0.52534900	0.28754700	H	-1.64967500	-3.49407900	-3.81539900
C	0.66983900	1.37914800	1.11398400	C	-2.98799900	-1.13542600	-3.92712800
H	1.40429000	1.05304100	1.85917600	H	-2.48339700	-1.02556400	-4.91207700
C	-0.92554100	-2.40410700	2.47628300	H	-3.78943900	-1.87254000	-4.07736800
H	-1.47930700	-3.11545100	1.86019400	H	-3.44307900	-0.14508800	-0.71912300
C	0.25609100	2.74900800	1.10979900	C	-1.03434300	-0.28758700	-2.67814100
C	-0.69028600	3.22943100	0.17164600	H	-0.66098000	0.06532600	-3.66480200
C	0.79271100	3.65192100	2.05734400	H	-1.56958000	0.56279300	-2.20667600
C	-1.08065200	4.55992300	0.19183300	H	-0.14022700	-0.52295400	-0.07372400
H	-1.10163000	2.53796600	-0.55579500	C	3.82532900	-0.66909100	-0.78436100
C	0.39533300	4.98204400	2.06767400	C	5.20415700	-0.44365500	-0.58854600
H	1.52067800	3.29235700	2.78112900	C	3.03443700	0.44943700	-1.13297100
C	-0.54294200	5.44473400	1.13672200	C	5.76011900	0.84427900	-0.65287300
H	-1.80864900	4.91764100	-0.53150500	H	5.86727300	-1.26015400	-0.39871100
H	0.81396900	5.66513700	2.80179600	C	3.56907500	1.74497200	-1.20645600
H	-0.85310200	6.48564300	1.14699500	H	1.99605500	0.31806300	-1.38269600
C	-1.10685700	-2.42451000	3.89729300	C	4.93186300	1.93432100	-0.64695600
C	-1.98884500	-3.36975600	4.47010300	H	5.36260500	2.92434700	-1.03499100
C	-0.43804400	-1.50998500	4.74591100	C	-3.43444900	-0.76495200	-0.84911900
C	-2.19544100	-3.39759600	5.84294000	C	-4.67789600	-0.42394100	-1.42370500
H	-2.50734700	-4.07262400	3.82202700	C	-3.02828800	-0.02763700	-0.28792300
C	-0.65088700	-1.54643000	6.11589800	C	-5.47280100	0.61259100	-0.90787800
H	0.23158700	-0.78034200	4.30253400	H	-5.04172000	-0.94263200	-2.28817700
C	-1.52882100	-2.48722600	6.67233700	C	-3.80382400	1.01657500	0.81625800
H	-2.87720300	-4.12611800	6.27316400	H	-2.09727500	-0.24931100	-0.77506700
H	-0.13748500	-0.83829600	6.76093800	C	-5.02598300	1.32946900	0.20920400
H	-1.69446300	-2.50791400	7.74581400	H	-5.65092800	2.10752100	0.63015600
C	3.48990500	-2.83458000	0.70545400	C	-3.32813000	1.78295200	1.99995500
C	3.49996900	-2.85816900	-2.07509100	C	-2.66028600	1.13290700	3.05618200
C	2.86439100	-2.07956900	-3.26681600	C	-3.51208200	3.17717000	2.07130800
H	1.77285000	-1.94785600	-3.13619300	C	-2.16926300	1.86311400	4.14206500
H	3.32036000	-1.07532600	-3.39058600	H	-2.52839200	0.05962500	3.04906100
H	3.01958600	-2.61788200	-4.22746900	C	-3.02164300	3.90222500	3.16148600
C	5.00801800	-2.98723800	-2.42744500	H	-4.00215200	3.71243700	1.26797700
H	5.61337600	-3.44801900	-1.63386300	C	-2.34629900	3.24693900	4.19287800
H	5.13822500	-3.62203900	-3.33109100	H	-1.65294800	1.35492300	4.94608400
H	5.45538000	-2.00418300	-2.68013700	H	-3.15306600	4.97585100	3.19905000
C	2.87433800	-4.27280000	-2.11016100	H	-1.96118900	3.81151600	5.03200800
H	2.89362800	-4.69196700	-3.13983800	C	-6.77728300	0.94193100	-1.53623300
H	3.44581200	-4.99007500	-1.49310000	C	-7.16078000	2.28288700	-1.72640700
H	1.81189300	-4.25017100	-1.78809700	C	-7.64985400	-0.08180200	-1.95182100
C	4.82499800	-3.61551100	0.82048900	C	-8.38868800	2.59028900	-2.32030000
H	4.86206200	-4.48164100	0.13509700	H	-6.50414900	3.09191200	-1.43142100
H	5.72438200	-2.99729100	0.69477400	C	-8.87677000	0.23151200	-2.54452600
H	4.92262000	-4.04822500	1.84054300	H	-7.39072800	-1.12279600	-1.80315600
C	2.38092200	-3.87564500	1.07227300	C	-9.24575200	1.56592400	-2.72891800
H	2.39298200	-4.76727800	0.42363700	H	-8.67436000	3.62395700	-2.46672700
				H	-9.54349200	-0.56138700	-2.85806900

H	-10.19590300	1.80618200	-3.18820600
C	2.70855100	2.89693400	-1.58325100
C	1.74027200	2.76837500	-2.59825700
C	2.85257600	4.13835400	-0.93495300
C	0.94188400	3.85811800	-2.95742200
H	1.61353800	1.83307900	-3.12872300
C	2.05413100	5.22565800	-1.30134400
H	3.56971600	4.26318700	-0.13347300
C	1.10181300	5.08666400	-2.31321400
H	0.20095400	3.75052000	-3.73895500
H	2.16707000	6.17440900	-0.79297300
H	0.48076200	5.92832900	-2.59089400
C	7.21408300	1.04824000	-0.43117200
C	7.67259900	2.12732700	0.34761800
C	8.15565400	0.16731100	-0.99648100
C	9.04188500	2.31745100	0.55704300
H	6.97168000	2.81308600	0.80717500
C	9.52372900	0.36270900	-0.78426100
H	7.83522500	-0.66102800	-1.61608900
C	9.96646000	1.43615900	-0.00804400
H	9.38609400	3.14730000	1.16068900
H	10.24140000	-0.31699400	-1.22525100
H	11.02597700	1.58539500	0.15507200

bis-benzaldehyde quintet

Cr	0.28670900	-1.19359600	0.25986700
O	1.86125900	-1.94499200	-0.19266700
O	-1.35553200	-2.01633000	0.13317100
C	3.27223300	-2.20878700	-0.12597500
C	-2.50747400	-2.30842100	-0.67079600
O	0.14179400	-0.79280600	2.19573900
O	0.11070500	0.66476200	-0.27414900
C	0.40853800	1.70377700	0.40168800
H	1.10492500	1.61081400	1.24351900
C	-0.69578200	-1.30505300	3.00226200
H	-1.13780700	-2.27172300	2.74909300
C	-0.08661100	3.00669600	0.06102100
C	-0.97454500	3.18944300	-1.02515000
C	0.34988100	4.13736000	0.78684900
C	-1.39829100	4.46416400	-1.37114900
H	-1.30690000	2.31795400	-1.57904300
C	-0.07997500	5.40944100	0.43247500
H	1.03340900	4.00249800	1.62197200
C	-0.95278500	5.57965200	-0.64882000
H	-2.07872200	4.59760300	-2.20769200
H	0.26326500	6.27324700	0.99493200
H	-1.28656300	6.57546800	-0.92601500
C	-1.08122300	-0.68465600	4.23883400
C	-2.04462500	-1.31672100	5.05655400
C	-0.51569300	0.53917600	4.66541300
C	-2.43480300	-0.73998000	6.25804900
H	-2.48362700	-2.25654300	4.72970800
C	-0.90957100	1.10653800	5.86904900
H	0.22361200	1.02103800	4.03419600
C	-1.86959900	0.47327100	6.66952300
H	-3.18073200	-1.23003600	6.87764700
H	-0.47293100	2.04810800	6.19130700
H	-2.17432700	0.92297800	7.61037400
C	3.52361500	-2.59560900	1.43211900
C	3.54584000	-3.31985300	-1.25203200
C	2.93856200	-2.84137700	-2.60592400
H	1.84433200	-2.67834500	-2.53171200
H	3.40711800	-1.89721800	-2.95348000
H	3.10342300	-3.59445000	-3.40753400
C	5.04491200	-3.60098500	-1.54814700
H	5.63347600	-3.85493200	-0.65428400
H	5.14500100	-4.45997000	-2.24716800
H	5.52982400	-2.74060800	-2.05369300
C	2.85876700	-4.66905500	-0.93258900

H	2.84693300	-5.33148100	-1.82560900
H	3.40289000	-5.23562500	-0.15512800
H	1.80372000	-4.51950900	-0.62451000
C	4.81501200	-3.38805000	1.76314200
H	4.82123900	-4.39256500	1.30391300
H	5.74464900	-2.85545100	1.51694300
H	4.87591000	-3.56821700	2.85912000
C	2.35607600	-3.45239500	2.02301300
H	2.34410000	-4.48625900	1.63818300
H	2.45895400	-3.55597100	3.12548000
H	1.35927800	-3.00800300	1.84737800
C	3.56084000	-1.29634100	2.28756900
H	4.49555800	-0.72317200	2.12021600
H	2.70305700	-0.63641000	2.04437900
H	3.52431300	-1.51880200	3.37630600
C	-1.96762600	-2.44633600	-2.18632600
C	-3.14742700	-3.61985800	0.04603600
C	-2.05295800	-4.60414800	0.57166900
H	-1.33297500	-4.11436100	1.25751700
H	-2.51459000	-5.43337000	1.15148600
H	-1.48785200	-5.09630000	-0.23655000
C	-3.94864700	-3.19191100	1.31146400
H	-3.34632700	-2.51875100	1.95534300
H	-4.88887400	-2.66694900	1.04274500
H	-4.24745300	-4.07038000	1.92424900
C	-4.10940600	-4.47711100	-0.81358200
H	-4.51240800	-5.31875900	-0.20832200
H	-4.99697700	-3.92349100	-1.15792900
H	-3.59761800	-4.95374200	-1.66829100
C	-1.00854300	-3.64771300	-2.35867300
H	-0.45667300	-3.58082400	-3.32202700
H	-0.25023900	-3.56025800	-1.55006700
H	-1.55044000	-4.61026400	-2.39502900
C	-3.05169300	-2.54601700	-3.29539400
H	-2.58210700	-2.79055100	-4.27344000
H	-3.80509300	-3.32674700	-3.11577600
H	-3.56596700	-1.57510500	-3.45156500
C	-1.12958600	-1.18587700	-2.54664100
H	-0.84013200	-1.18792000	-3.62074000
H	-1.69541300	-0.24928900	-0.26045300
H	-0.18315700	-1.15525500	-1.97435700
C	3.99528700	-0.89524000	-0.53463000
C	5.38721400	-0.71446700	-0.38827100
C	3.26524600	0.10222200	0.10647900
C	6.01369300	0.50039900	-0.71217400
H	6.00495300	-1.51083800	-0.02989000
C	3.86923300	1.39604100	-1.42893200
H	2.21871100	0.05484200	-1.32701100
C	5.24264900	1.55701700	-1.21301500
H	5.72255200	2.48808400	-1.48974800
C	-3.47239800	-1.09232800	-0.56102200
C	-4.74917000	-1.08838700	-1.16383200
C	-3.11773300	0.04542600	0.20468100
C	-5.62988000	-0.00451000	-1.02938700
H	-5.07607000	-1.91415000	-1.76226100
C	-3.98378200	1.14413800	0.34579900
H	-2.16128500	0.09420700	0.69811300
C	-5.23811000	1.10682700	-0.27542300
H	-5.93041700	1.92854000	-0.13872000
C	-3.58345600	2.33004300	1.15010300
C	-2.86492900	2.17505200	2.35039300
C	-3.91590100	3.63033900	0.72267800
C	-2.47633600	3.29314800	3.09429500
H	-2.62033800	1.19000800	2.72163000
C	-3.53041100	4.74438000	1.47391900
H	-4.44861400	3.78835200	-0.20643100
C	-2.80756000	4.57629600	2.65608000
H	-1.92186300	3.16588200	4.01402000
H	-3.78020600	5.73999200	1.13086300
H	-2.50284200	5.44054200	3.23176400
C	-6.96786300	-0.03922800	-1.67281400

C	-7.47731700	1.09966200	-2.32455800	C	-2.50598500	-3.36190300	2.05797400
C	-7.74687000	-1.21154100	-1.64086100	H	-1.45328900	-3.01047800	2.08260900
C	-8.73653100	1.06379600	-2.93124500	H	-3.14800900	-2.56739400	2.49218600
H	-6.89505300	2.01109600	-2.37898700	H	-2.57160100	-4.23557800	2.74307400
C	-9.00561600	-1.24142100	-2.24867300	C	-4.39590100	-4.31649100	0.77775400
H	-7.38988800	-2.09838000	-1.13194100	H	-4.88038600	-4.58873400	-0.17037600
C	-9.49985500	-0.10529300	-2.89345100	H	-4.36874400	-5.24685400	1.38625100
H	-9.11933000	1.94258000	-3.43395700	H	-5.05720000	-3.61674400	1.32786700
H	-9.59975700	-2.14557200	-2.21664200	C	-2.02881800	-4.89924800	0.17298500
H	-10.47445100	-0.13073200	-3.36352600	H	-1.94914400	-5.67282500	0.96772500
C	3.06458000	2.50267800	-2.00509200	H	-2.40208000	-5.43056100	-0.71875700
C	2.10931600	2.24795900	-3.00743000	H	-1.00469000	-4.53136300	-0.02725200
C	3.24372200	3.82372600	-1.55444900	C	-4.06628500	-3.67339500	-2.42490000
C	1.35904200	3.29451700	-3.55151600	H	-3.83981000	-4.71009000	-2.12630500
H	1.95517500	1.24374800	-3.38213100	H	-5.08914600	-3.40973000	-2.11389000
C	2.48814000	4.86587600	-2.09982700	H	-4.10264100	-3.69704900	-3.53642200
H	3.95544800	4.04671000	-0.76943300	C	-1.65348600	-3.11813500	-2.60094300
C	1.54999200	4.60229600	-3.10006400	H	-1.33405000	-4.11368800	-2.24986100
H	0.62732600	3.09093500	-4.32250900	H	-1.75579200	-3.20520900	-3.70500100
H	2.62573700	5.87797400	-1.74203400	H	-0.83413000	-2.39012700	-2.42260700
H	0.96347700	5.41009200	-3.51808800	C	-3.34155300	-1.31327400	-2.64807600
C	7.47922500	0.66123500	-0.53556900	H	-4.38110800	-0.99068400	-2.43964800
C	8.00696300	1.84653100	0.01020100	H	-2.65668000	-0.51205600	-2.32759600
C	8.36294700	-0.36832300	-0.91133300	H	-3.26221800	-1.39539700	-3.75436400
C	9.38712700	1.99547600	0.17735300	C	2.61598300	-2.86916200	1.67874800
H	7.35144000	2.64992600	0.32249500	C	3.11344800	-3.69735100	-0.93325700
C	9.74221800	-0.21358900	-0.74249800	C	1.87343400	-4.58587300	-1.26090300
H	7.98900000	-1.28459400	-1.35107500	H	1.01555300	-3.98386700	-1.61860100
C	10.25383100	0.96667600	-0.19843000	H	2.10912000	-5.30569100	-2.07524300
H	9.78462400	2.90842900	0.60165500	H	1.54468500	-5.21305300	-0.41746000
H	10.41517000	-1.00845200	-1.03720000	C	3.54228100	-3.09744000	-2.30616600
H	11.32188600	1.08422300	-0.06844000	H	2.78564800	-2.36984000	-2.67148100
				H	4.52651000	-2.58732100	-2.24279700
				H	3.65301400	-3.88686500	-3.08157300
				C	4.24181100	-4.66204900	-0.50011700
				H	4.44553700	-5.39972800	-1.30711000
				H	5.19928200	-4.14427000	-0.32291800
				H	3.95788800	-5.26361500	0.38237400
				C	1.66612700	-4.06689100	1.91150200
				H	1.36765400	-4.13645200	2.98080200
				H	0.73392400	-3.94816100	1.32851600
				H	2.15279000	-5.03168900	1.67540200
				C	3.92363600	-3.16758800	2.46466300
				H	3.68695700	-3.57966800	3.47036200
				H	4.57553900	-3.91003100	1.98009700
				H	4.50082000	-2.24100300	2.66569900
				C	1.96065900	-1.67193900	2.41926600
				H	1.95970200	-1.82810200	3.52081200
				H	2.50845700	-0.72737100	2.22149900
				H	0.89722800	-1.55741400	2.12543400
				C	-3.76372300	-1.33749900	0.20081900
				C	-5.16179100	-1.36561400	0.01255800
				C	-3.23168200	-0.25169800	0.93519300
				C	-5.99063500	-0.32776900	0.46831600
				H	-5.62262900	-2.18444900	-0.50262700
				C	-4.04533700	0.79168400	1.40350700
				H	-2.17661100	-0.20743100	1.15575600
				C	-5.42091700	0.75413600	1.15081200
				H	-6.05587000	1.54631800	1.52925200
				C	3.76508200	-1.32132700	-0.09619300
				C	5.13264800	-1.40855100	0.25087000
				C	3.35406000	-0.15229900	-0.78426900
				C	6.02508800	-0.34773100	0.02763700
				H	5.53415400	-2.29465100	0.69795700
				C	4.24470900	0.89992600	-1.05297500
				H	2.34439600	-0.05712000	-1.15219700
				C	5.56821200	0.80816100	-0.61326500
				H	6.26230600	1.61100100	-0.83226900
				C	3.80766700	2.67753600	-1.83947100
				C	3.08830500	1.90668200	-3.03610800
				C	4.13087200	3.37904700	-1.41612800

benzaldehyde transition state triplet

Cr	0.00272000	-1.02394700	-0.26459400
O	-1.48218900	-2.00928300	-0.13604300
O	1.47427000	-2.04207400	-0.30634100
C	-2.83352900	-2.45469700	-0.34061800
C	2.77364600	-2.50292800	0.10913800
O	-0.63655700	0.37946300	-1.36972100
O	0.61140100	0.44079700	0.77658900
C	0.09213100	1.64927900	0.65004100
H	-0.97599400	1.76410900	0.85169600
C	-0.19754000	1.62350900	-1.26853100
H	0.84854300	1.80861900	-1.52858800
C	0.90725400	2.79650800	1.11042200
C	2.25815800	2.63072100	1.45340300
C	0.32684700	4.07057600	1.22086100
C	3.00939500	3.71576400	1.89675800
H	2.69732500	1.64198700	1.39082700
C	1.08317000	5.15672600	1.65505600
H	-0.71903100	4.20652100	0.96215900
C	2.42761500	4.98311300	1.99264900
H	4.05195800	3.57343100	2.16882900
H	0.62154500	6.13702600	1.73685800
H	3.01699100	5.82904400	2.33601900
C	-1.12077200	2.71840400	-1.64389100
C	-0.61055900	3.96996300	-2.02148300
C	-2.51303600	2.54702000	-1.56645400
C	-1.47036500	5.02461200	-2.32345900
H	0.46432400	4.11583400	-2.06790900
C	-3.37094600	3.60108400	-1.86536100
H	-2.91083800	1.58320300	-1.27175000
C	-2.85309800	4.84371000	-2.24486300
H	-1.06133700	5.98676600	-2.61956500
H	-4.44604400	3.45550200	-1.80093500
H	-3.52445900	5.66586300	-2.47753400
C	-2.99279800	-2.65849600	-1.94970200
C	-2.96109600	-3.74328100	0.61441100

C	2.68612000	3.01790700	-3.78314500	H	0.33326800	2.56161900	-4.06052300
H	2.84253100	0.91439200	-3.39387200	C	-3.41243900	3.09187400	-3.25254700
C	3.72173500	4.48723000	-2.16339400	H	-3.02814100	2.03056200	-1.43177600
H	4.68896400	3.53745400	-0.50215200	C	-2.88441900	3.58965600	-4.44518900
C	3.00228000	4.30699000	-3.34713800	H	-1.11120100	3.78125900	-5.65914000
H	2.12794500	2.87944400	-4.69994400	H	-4.46448100	3.23465200	-3.02008200
H	3.96414700	5.48625900	-1.82501000	H	-3.52293900	4.12261500	-5.14465600
H	2.68610400	5.16609800	-3.92440400	C	-3.22071000	-2.51513200	-1.90440400
C	7.44746400	-0.45963000	0.43849400	C	-2.95642100	-3.90510100	0.48733100
C	8.09740900	0.62443200	1.05764600	C	-2.32634600	-3.73418600	1.90417500
C	8.16752500	-1.64850600	0.21465500	H	-1.28997600	-3.35061000	1.85685400
C	9.43628100	0.51843200	1.44634200	H	-2.91939500	-3.03555500	2.53104400
H	7.56516600	1.54675600	1.25494200	H	-2.29612800	-4.70034200	2.45374400
C	9.50640500	-1.74863100	0.60484900	C	-4.40961100	-4.38944000	0.74889000
H	7.70110200	-2.49302700	-0.27722500	H	-4.96747700	-4.64220500	-0.16427300
C	10.13999600	-0.66676300	1.22050800	H	-4.39466600	-5.32475200	1.35048000
H	9.92762300	1.35521900	1.92580300	H	-4.99218900	-3.65725700	1.34133000
H	10.05416700	-2.66491100	0.42622300	C	-2.18828800	-5.06540400	-0.19385900
H	11.17646200	-0.74656800	1.52187500	H	-2.09061300	-5.93595300	0.49061200
C	-3.45488400	1.92479900	2.15585100	H	-2.71280100	-5.45025100	-1.08552600
C	-2.51274200	1.69282700	3.17522700	H	-1.16615600	-4.76126800	-0.48523900
C	-3.81288100	3.24920000	1.84496800	C	-4.43339700	-3.38263200	-2.33464900
C	-1.93584800	2.76559100	3.86144000	H	-4.22946900	-4.46467300	-2.25717600
H	-2.22440900	0.68305000	3.43990500	H	-5.36456700	-3.14397400	-1.79948500
C	-3.23527100	4.31812300	2.53639200	H	-4.66221500	-3.20931400	-3.40944000
H	-4.52302000	3.45667900	1.05422200	C	-2.02949100	-2.99626700	-2.79161900
C	-2.29744600	4.07677400	3.54328500	H	-1.72837900	-4.03512000	-2.57563600
H	-1.20669800	2.58006100	4.63937500	H	-2.30181200	-2.97427400	-3.86981900
H	-3.50834600	5.33475100	2.28506200	H	-1.13954500	-2.34444500	-2.68559300
H	-1.84605500	4.90600200	4.07233700	C	-3.53125000	-1.06671700	-2.38005600
C	-7.45555000	-0.37721500	0.23237500	H	-4.55637700	-0.74826900	-2.10262600
C	-8.15330100	0.77695500	-0.17060500	H	-2.82210100	-0.34941000	-1.925430700
C	-8.16843600	-1.57873100	0.40588100	H	-3.46994900	-0.96914800	-3.48608500
C	-9.53241700	0.72768000	-0.39538700	C	2.38551500	-2.87036800	1.25801000
H	-7.62961800	1.71170100	-0.32806400	C	3.14207600	-3.39952700	-1.36905100
C	-9.54760100	-1.62194200	0.18035200	C	1.93630700	-4.22496900	-1.92587600
H	-7.66269600	-2.47918500	0.73174600	H	1.10782300	-3.58082200	-2.28530400
C	-10.22887600	-0.47027000	-0.22010100	H	2.24979200	-4.83631600	-2.80041800
H	-10.06092200	1.61862700	-0.70909400	H	1.53531100	-4.95435400	-1.20339100
H	-10.08905300	-2.54876200	0.31945800	C	3.70721800	-2.60319200	-2.60419200
H	-11.29647800	-0.50609500	-0.39445000	H	2.99490800	-1.85463000	-2.94419000
----				H	4.68166800	-2.15533000	-2.37968600
benzaldehyde diolate triplet				H	3.89084300	-3.32347500	-3.45971600
----				C	4.21638400	-4.43571400	-0.95646900
Cr	-0.11018300	-1.05714000	-0.61126400	H	4.45546400	-5.09803700	-1.81736200
O	-1.41288300	-2.20109000	-0.29688900	H	5.17725300	-3.97691600	-0.67490900
O	1.45513800	-2.81445200	-0.74779100	H	3.86347200	-5.11128900	-0.15775800
C	-2.83282100	-2.52412700	-0.32429900	C	1.44290500	-4.09126800	-1.25385300
C	2.70210400	-2.33429200	-0.22891800	H	1.03036000	-4.28264000	2.26892600
O	-0.42775400	0.03198700	-1.97698300	H	0.58867200	-3.90743300	0.58055800
O	0.00436800	0.42691900	0.40528400	H	1.96568500	-5.02141000	0.96407600
C	-0.52042500	1.60689800	-0.18599500	C	3.61528200	-3.24635000	2.12997000
H	-1.60201600	1.64543500	0.00936800	H	3.28784600	-3.74737500	3.06747600
C	-0.30518300	1.44315100	-1.70888700	H	4.30841400	-3.94495200	1.63542900
H	0.72076600	1.73297700	-1.759877400	H	4.17246800	-2.34552100	2.46124200
C	0.10796100	2.83966000	0.44218700	C	1.63923100	-1.75997800	2.05021200
C	1.13331900	2.70844400	1.38416800	H	1.51749700	-2.03915600	3.12008500
C	-0.36691600	4.12082300	0.13014900	H	2.18874200	-0.79599800	2.01959100
C	1.66655400	3.83526600	2.01173700	H	0.61759400	-1.60639700	1.65334300
H	1.48992200	1.71631400	1.63439500	C	-3.56000600	-1.41503900	0.48000600
C	0.17706900	5.24701700	0.74674500	C	-4.95593400	-1.22044400	0.42400100
H	-1.17189900	4.23953500	-0.58965000	C	-2.82703500	-0.56541300	1.33635700
C	1.19233600	5.10815200	1.69527300	C	-5.58037000	-0.15691400	1.09707600
H	2.45557700	3.71543400	2.74983600	H	-5.57217800	-1.87532100	-0.15793900
H	-0.20125800	6.23392300	0.49320400	C	-3.42341200	0.51865000	1.99613600
H	1.60881200	5.98539100	2.18313900	H	-1.77963200	-0.74599900	1.50226000
C	-1.23230400	2.21439100	-2.62814000	C	-4.80170800	0.72243800	1.86154400
C	-0.71752600	2.71693700	-3.83003900	H	-5.27613200	1.53949000	2.39153400
C	-2.59382500	2.40889300	-2.35294300	C	3.70516900	-1.14645800	-0.16503300
C	-1.53220800	3.39907500	-4.73303200	C	5.05117200	-1.32256000	0.23075200
				C	3.32196200	0.15610400	-0.56979200

C	5.96127600	-0.25535700	0.27447700	H	1.70878600	-3.84607100	-0.38479400
H	5.41331500	-2.28132600	0.53955800	H	-0.20053300	-5.15184000	3.24407000
C	4.22702500	1.23168100	-0.54646000	H	1.40144300	-5.56966400	1.38745400
H	2.31896600	0.35249800	-0.90940200	C	-0.23446900	4.41728800	1.57194700
C	5.53705300	1.02023500	-0.10799700	C	0.22002900	5.41471100	0.69696600
H	6.24157500	1.84370700	-0.11064300	C	-1.43975300	4.60746200	2.25992900
C	3.81695300	2.57904600	-1.00377500	C	-0.52710000	6.57662600	0.50444300
C	3.16382600	2.74492100	-2.23656500	H	1.16033300	5.27720100	0.17067800
C	4.10224500	3.71288600	-0.22271000	C	-2.18776700	5.76924400	2.06280700
C	2.76690500	4.01715800	-2.65999700	H	-1.79308400	3.84231000	2.94609300
H	2.96665400	1.89052800	-2.87245600	C	-1.73249500	6.75546500	1.18625000
C	3.70672100	4.98344800	-0.65150900	H	-0.16789500	7.34085900	-0.17924700
H	4.60845500	3.61138900	0.72936900	H	-3.12629500	5.90230700	2.59400100
C	3.03236100	5.13455200	-1.86520200	H	-2.31552500	7.65953500	1.03384500
H	2.25818900	4.13817900	-3.60722800	C	-3.21105900	2.68650000	-1.30332100
H	3.91460000	5.84997700	-0.03731900	C	-2.88851700	1.30575700	-3.68231200
H	2.72144900	6.11804100	-2.19275800	C	-2.26725800	-0.00284800	-4.26463700
C	7.36315300	-0.47864700	0.71082200	H	-1.26301100	-0.20913800	-3.85575500
C	7.99907300	0.43851400	1.56857800	H	-2.91168500	-0.88350600	-4.05863500
C	8.07726700	-1.61042900	0.27348000	H	-2.16862700	0.04471900	-5.37103400
C	9.31830100	0.22527200	1.97984300	C	-4.35333600	1.32016100	-4.20697700
H	7.47063300	1.31041500	1.93360600	H	-4.82677400	2.31487900	-4.17013900
C	9.39645500	-1.81821400	0.68743700	H	-4.37928400	1.04932200	-5.28555100
H	7.62151500	-2.32462800	-0.40110800	H	-4.99420100	0.58524300	-3.68578800
C	10.01625100	-0.90175800	1.53993800	C	-2.13839500	2.47642200	-4.36342600
H	9.79870700	0.93315500	2.64289600	H	-2.06205100	2.32094500	-5.46147000
H	9.93970800	-2.68909300	0.34396300	H	-2.67978300	3.43374800	-4.24842800
H	11.03747400	-1.06471700	1.85933500	H	-1.10629100	2.57808900	-3.97214100
C	-2.59339400	1.45706700	2.79428400	C	-4.49756100	3.37403900	-1.83269900
C	-1.56413300	0.97783600	3.62709600	H	-4.30467300	3.92967400	-2.77078200
C	-2.79231800	2.84658800	2.68914000	H	-5.34454000	2.69175000	-1.99225500
C	-0.75591000	1.86999600	4.33783800	H	-4.85241800	4.14303900	-1.11194200
H	-1.38953600	-0.08531000	3.73520100	C	-2.10571700	3.78320200	-1.34993500
C	-1.98088300	3.73393800	3.40217900	H	-1.82728400	4.09980600	-2.36545800
H	-3.55550300	3.24672700	2.03344000	H	-2.44472100	4.70487800	-0.82964600
C	-0.96463500	3.24634600	4.22640300	H	-1.18974300	3.44724500	-0.83357800
H	0.03499700	1.49360000	4.97352700	C	-3.41302500	2.42334100	0.21394200
H	-2.13229100	4.80123000	3.30576200	H	-4.29010800	1.79345100	0.44266800
H	-0.33297500	3.93549300	4.77170700	H	-2.50774400	1.95522800	0.63852100
C	-7.04787300	0.04010700	0.99029300	H	-3.58291200	3.37125900	0.76872600
C	-7.58485600	1.32880100	0.81069300	C	2.48198700	-0.08903500	-3.23599700
C	-7.92408900	-1.05927000	1.06312800	C	2.99415200	2.29642300	-1.90542500
C	-8.96717300	1.51102800	0.70622400	C	1.71133600	3.14036900	-2.15631100
H	-6.93520900	2.19178200	0.73361700	H	0.90950500	2.88764900	-2.48667100
C	-9.30557700	-0.87102200	0.95880900	H	1.91546700	4.22557700	-2.02692700
H	-7.54197500	-2.06085600	1.21697800	H	1.32477800	3.04474000	-3.18489800
C	-9.82664500	0.41253000	0.78035100	C	3.55153800	2.77801700	-0.53758400
H	-9.37196800	2.50474000	0.56409000	H	2.91396300	2.41845600	0.28578100
H	-9.97283400	-1.72108600	1.01949600	H	4.58339000	2.41006400	-0.36092800
H	-10.89638800	0.55591500	0.69940300	H	3.59829800	3.88726200	-0.47547100
----				C	4.01654900	2.76638200	-2.97372100
bis-benzophenone singlet				H	4.15100700	3.86875500	-2.90830500
----				H	5.02705300	2.35434300	-2.83072200
Cr	-0.16463200	1.07820200	-0.43380100	H	3.67460000	2.58113900	-4.00556100
O	-1.32221000	1.21758200	-1.79732300	C	1.49180300	0.62626400	-4.18233000
O	1.40401100	0.53818400	-1.17021300	H	1.13864000	-0.05598100	-4.98661300
C	-2.74143800	1.33095100	-2.07054900	H	0.60413400	0.96540000	-3.62168500
C	2.66939500	0.70081400	-1.84077200	H	1.94864500	1.48673900	-4.70260100
O	0.48500000	2.20893600	0.96445900	C	3.78004800	-0.37273300	-4.04204500
O	-0.98494700	0.00757300	0.81688900	H	3.52927500	-0.78187300	-5.04534800
C	-1.37744500	-0.97972800	1.52306700	H	4.39777100	0.52005100	-4.22022500
C	0.58971000	3.17911800	1.76443500	H	4.40287800	-1.14998500	-3.55295000
C	-0.63495700	-2.24258000	1.50883000	C	1.85936100	-1.49044200	-2.95374300
C	0.28198900	-2.49144400	0.46782300	H	1.80297100	-2.10114900	-3.88170700
C	-0.79507600	-3.22369400	2.51079700	H	2.46226300	-2.06391400	-2.21921500
C	1.00759100	-3.67587900	0.42741300	H	0.82112600	-1.40402700	-2.57243100
H	0.41681400	-1.73929500	-0.29861600	C	-3.38687100	0.02735100	-1.51560100
C	-0.07105700	-4.41094700	2.45974400	C	-4.75500100	-0.08483900	-1.18691600
H	-1.47043900	-3.04353800	3.34021600	C	-2.61798700	-1.16166600	-1.45886400
C	0.83360500	-4.64395400	1.42009300	C	-5.32288000	-1.30373000	-0.78404300
				H	-5.40760100	0.76091200	-1.24624700

C	-3.19021800	-2.40926000	-1.15987400	C	3.32979000	1.90551000	4.00843300
H	-1.56555600	-1.13431600	-1.69830600	H	2.32293600	1.22061400	2.22755000
C	-4.54280800	-2.46560400	-0.80394700	C	2.60042000	4.05439900	4.84786800
H	-4.99260000	-3.411453300	-0.54136100	H	1.03540600	5.02538600	3.74019400
C	3.71628600	-0.05054100	-0.96018500	C	3.43063300	2.93469300	4.95183000
C	5.08923400	-0.07934200	-1.28783200	H	3.97748900	1.03555800	4.07690300
C	3.32465100	-0.74240100	0.21592100	H	2.67812800	4.85781400	5.57545400
C	6.02483200	-0.78130000	-0.51339500	H	4.15466700	2.86626900	5.75914200
H	5.45641500	0.43649500	-2.14982300				
C	4.23702400	-1.49834600	0.97412200	----			
H	2.30061100	-0.72620900	0.54216300	bis-benzophenone triplet			
C	5.58904800	-1.49267300	0.60913900	----			
H	6.30694200	-2.05282700	1.19565100	Cr	0.06775700	-1.08120500	-0.61888400
C	3.77826800	-2.33495700	2.12012700	O	1.25232900	-1.17508700	-1.98627800
C	2.78293200	-1.87845700	3.00556100	O	-1.53722700	-0.65062200	-1.30833000
C	4.32616000	-3.61695700	2.32734800	C	2.66489700	-2.12064800	-2.30091100
C	2.36835900	-2.66910500	4.08075200	C	-2.81737900	-0.71948000	-1.95515400
H	2.32498600	-0.91288800	2.87659900	O	-0.33677400	-2.38990600	0.69752300
C	3.90263300	-4.40729000	3.40002100	O	1.04039100	-0.04046400	0.76907000
H	5.06760300	-4.01853100	1.64848900	C	1.44847000	0.89134200	1.52502800
C	2.92807700	-3.93198200	4.27876500	C	-0.33474000	-3.15329600	1.73266100
H	1.60400200	-2.30533300	4.75525700	C	0.68000800	2.14233500	1.63160000
H	4.32722600	-5.39198100	3.54645000	C	-0.27009000	2.44815300	0.63616500
H	2.59919300	-4.54615300	5.10690900	C	0.84032700	3.04828000	2.70135500
C	7.46074800	-0.78747800	-0.89191100	C	-1.01921400	3.61615500	0.69630500
C	8.45834500	-0.63698600	0.08954300	H	-0.40540800	1.76052200	-0.18859700
C	7.84619800	-0.94354500	-2.23698700	C	0.09331300	4.22159600	2.75383200
C	9.80985900	-0.64071000	-0.26874600	H	1.53146700	2.81789200	3.50442800
H	8.19218900	-0.49988500	1.13022900	C	-0.83801200	4.51291600	1.75317300
C	9.19918300	-0.94717900	-2.58939500	H	-1.74215100	3.83042000	-0.08580900
H	7.10295900	-1.07951200	-3.01269000	H	0.22441300	4.90345600	3.58947600
C	10.17997100	-0.79553700	-1.60661400	H	-1.42302700	5.42704800	1.80104300
H	10.57075700	-0.52016300	0.49152900	C	0.74373000	-4.17243000	1.87803200
H	9.48735900	-1.07112100	-3.62530500	C	0.88861500	-5.18795900	0.92046300
H	11.22676000	-0.79834900	-1.88171300	C	1.62183600	-4.15168000	2.97508100
C	-2.37942600	-3.65435100	-1.25831100	C	1.89860400	-6.14129400	1.04218900
C	-2.55290800	-4.70676200	-0.33792400	H	0.19301700	-5.23392800	0.08698300
C	-1.42865300	-3.80631300	-2.28788100	C	2.64001200	-5.09838900	3.08932600
C	-1.78793200	-5.87229600	-0.44017000	H	1.50584500	-3.38529600	3.73676500
H	-3.26498600	-4.62630500	0.47163000	C	2.78350200	-6.09451700	2.12147200
C	-0.66416900	-4.97245000	-2.38243100	H	1.99334900	-6.92287900	0.29305000
H	-1.28581400	-3.03178600	-3.03056700	H	3.31896200	-5.06018900	3.93738600
C	-0.84304200	-6.00424700	-1.45937900	C	3.57427500	-6.83424900	2.21176200
H	-1.92157000	-6.67055000	0.27833200	H	3.17564100	-2.62251900	-1.67870100
H	0.06635900	-5.07649500	-3.17419600	C	2.76931700	-1.03362900	-3.90774300
H	-0.24787600	-6.90514300	-1.53235200	C	2.08489200	0.29514000	-4.35777500
C	-6.73814000	-1.35855600	-0.34317000	H	1.08068800	0.41842700	-3.91461400
C	-7.24774000	-0.37534800	0.52546200	H	2.69922100	1.18001000	-4.08937400
C	-7.58446000	-2.39948600	-0.76744900	H	1.96394000	0.34331600	-5.46194400
C	-8.57483100	-0.43485300	0.96012700	C	4.22215500	-0.94471900	-4.45658300
H	-6.61361500	0.42643200	0.88354500	H	4.73800000	-1.91977800	-4.50860600
C	-8.91206900	-2.45257800	-0.33182800	H	4.21573500	-0.58359000	-5.50864400
H	-7.22379000	-3.16243300	-1.44587700	H	4.84409500	-0.23111800	-3.88445500
C	-9.40652500	-1.47197600	0.53155800	C	2.04698200	-2.16310600	-4.68197900
H	-8.95725900	0.32163600	1.63312200	H	1.93943900	-1.90892600	-5.75883100
H	-9.55839400	-3.25426100	-0.66507700	H	2.62757600	-3.10416900	-4.67267700
H	-10.43395600	-1.51620300	0.86896600	H	1.02713400	-2.33788000	-4.28240700
C	-2.62106200	-0.78578500	2.30318200	C	4.47570300	-3.21891000	-2.28151800
C	-2.87003900	0.45170500	2.92499000	H	4.28708900	-3.62889000	-3.26446400
C	-3.61204800	-1.78125700	2.38023500	H	5.29955500	-2.50066200	-2.39413100
C	-4.07764700	0.69425500	3.57247300	H	4.86313900	-4.03678500	-1.63519100
H	-2.09941500	1.21575600	2.89619700	C	2.09937500	-3.74220400	-1.82767500
C	-4.82580700	-1.53197900	3.01651500	H	1.83032100	-3.97753700	-2.86649600
H	-3.44236200	-2.74080300	1.90712200	H	2.46898200	-4.69909000	-1.40011800
C	-5.06636400	-0.29248900	3.61206100	H	1.17023300	-3.48460200	-1.28597600
H	-4.25051400	1.65652700	4.04718300	C	3.37778000	-2.50178500	-0.14344500
H	-5.59000500	-2.30435400	3.03445100	H	4.25925600	-1.89976400	0.13895500
H	-6.01500100	-0.09731600	4.10453900	H	2.47505000	-2.06436200	0.31954900
C	1.55660500	3.11579100	2.86253200	H	3.53819500	-3.49709100	0.32596100
C	2.40397300	1.99472300	2.97864500	C	-2.65743700	0.19502600	-3.27127400
C	1.67292600	4.15079700	3.81429200	C	-3.12722300	-2.30576800	-2.15220000

C	-1.84469400	-3.11299900	-2.52287500	C	0.69387600	6.03904500	-1.18589200
H	-1.01369900	-2.92113700	-1.82133400	H	1.79823300	6.62223400	0.56526800
H	-2.03750200	-4.20748300	-2.47880400	H	-0.23882700	5.19520000	-2.93108000
H	-1.49743900	-2.92731800	-3.55323800	H	0.09038200	6.93723300	-1.20060200
C	-3.61525500	-2.92173900	-0.81290100	C	6.64268900	1.39009200	-0.39702000
H	-2.87894500	-2.73032900	-0.01365200	C	7.17873200	0.34472700	0.37849400
H	-4.60000600	-2.52005800	-0.49996900	C	7.46798200	2.47771400	-0.73847200
H	-3.73917700	-4.02411600	-0.89136600	C	8.50860200	0.39066900	0.80600200
C	-4.18486000	-2.68919200	-3.22090300	H	6.56303100	-0.49672700	0.67147000
H	-4.29134700	-3.79544800	-3.26771600	C	8.79866300	2.51695600	-0.31087600
H	-5.19801700	-2.32481500	-2.99485600	H	7.08927500	3.28898500	-1.34731200
H	-3.89138700	-2.38834000	-4.24026500	C	9.31805700	1.47543600	0.46154600
C	-1.69763600	-0.42983000	-4.30927500	H	8.91041300	-0.41379300	1.40836200
H	-1.37546400	0.32204300	-5.06278400	H	9.42811800	3.35530900	-0.58001800
H	-0.78688200	-0.81041300	-3.81287700	H	10.34777500	1.50903600	0.79315100
H	-2.17185900	-1.24301700	-4.88707600	C	2.72961800	0.68787800	2.24081300
C	-3.98060600	0.55306800	-4.00247800	C	3.07948900	-0.60548700	2.67033000
H	-3.76347200	1.05966000	-4.96834100	C	3.66428100	1.72584800	2.41766900
H	-4.60433200	-0.32156900	-4.24188300	C	4.32294700	-0.85549400	3.24021200
H	-4.58854200	1.27256700	-3.41574900	H	2.36100600	-1.40882800	2.55606800
C	-2.01830800	1.56122300	-2.87460200	C	4.91432300	1.47043700	2.97630400
H	-1.95181500	2.24315000	-3.75077400	H	3.42749800	2.72628600	2.07689100
H	-2.61721300	2.08418200	-2.10040600	C	5.25021900	0.17971600	3.38950600
H	-0.98401900	1.43172300	-2.49359100	H	4.57150400	-1.86327600	3.56166200
C	3.29781200	0.05007900	-1.64328300	H	5.63301200	2.27954900	3.07390900
C	4.66566300	0.15385900	-1.31063600	H	6.22830300	-0.01901200	3.81899800
C	2.51494600	1.22065100	-1.49490100	C	-1.40011500	-3.05893100	2.71678700
C	5.22295900	1.34852600	-0.82821100	C	-2.38714500	-2.05502300	2.58928600
H	5.32837000	-0.67594900	-1.43289400	C	-1.51942300	-3.96663200	3.79867500
C	3.07550400	2.45309800	-1.11847400	C	-3.43170300	-1.95152400	3.49652800
H	1.46034500	1.19214700	-1.72484200	H	-2.31135700	-1.37697300	1.75071800
C	4.42966500	2.50017400	-0.76611900	C	-2.56440100	-3.85280400	4.70824000
H	4.87122800	3.43436000	-0.44438700	H	-0.79767200	-4.76783300	3.91357500
C	-3.83292700	-0.04102600	-0.98788300	C	-3.52663400	-2.84642500	4.56836600
C	-5.22035500	-0.03194900	-1.24564700	H	-4.17775200	-1.17101900	3.36935700
C	-3.39290000	0.62924500	0.18283700	H	-2.63620000	-4.56135600	5.52951600
C	-6.13364500	0.58404200	-0.37768200	H	-4.34336400	-2.76609500	5.28037700
H	-5.61444300	-0.49282700	-2.12627200				
C	-4.28794700	1.28953000	1.04450200	----			
H	-2.34494300	0.67505700	0.41982200	bis-benzophenone quintet			
C	-5.65967900	1.23664100	0.76493200	----			
H	-6.36386500	1.72058800	1.43036500	Cr	-0.03304500	-1.27941300	0.54678700
C	-3.79747000	2.06397200	2.22130300	O	-1.21550900	-1.27998500	1.94441800
C	-2.72431700	1.59833900	3.00570400	O	1.60908400	-0.81603000	1.17583800
C	-4.40508200	3.28661800	2.57197100	C	-2.61899000	-1.28425400	2.28819400
C	-2.29978800	2.31292300	4.12902500	C	2.86817500	-0.89825300	1.86406900
H	-2.21163600	0.68362300	2.76073900	O	0.33382700	-2.75615500	-0.64381600
C	-3.96756200	4.00476400	3.68886600	O	-1.01224300	-0.10606200	-0.91354600
H	-5.20803900	3.69783400	1.97372100	C	-1.44637600	0.88673900	-1.54935400
C	-2.92087700	3.51471000	4.47111400	C	0.08995500	-3.08558000	-1.88843400
H	-1.47806200	1.94034000	4.72695200	C	-0.64906900	2.13594800	-1.60168600
H	-4.43992800	4.94382200	3.94653200	C	0.32017500	2.35258600	-0.60687700
H	-2.58295400	4.07201100	5.33506700	C	-0.81146800	3.09827700	-2.61547000
C	-7.58777900	0.56040200	-0.67687600	C	1.09095200	3.50900600	-0.60854300
C	-8.52251500	0.30371300	0.34358600	H	0.45931400	1.60445500	0.16296700
C	-8.05344600	0.79400900	-1.98476700	C	-0.03664300	4.25583700	-2.61493700
C	-9.89136500	0.27972200	0.05959500	H	-1.52060500	2.92774900	-3.41783700
H	-8.19341200	0.10538900	1.35602900	C	0.91110400	4.46622000	-1.61051700
C	-9.42343200	0.76947000	-2.26284000	H	1.83143400	3.66292500	0.17055800
H	-7.36002100	1.01205200	-2.78750800	H	-0.16115400	4.98726300	-3.40803600
C	-10.34142000	0.51224800	-1.24205500	H	1.51467900	5.36952800	-1.61409100
H	-10.60355700	0.07742200	0.84913300	C	-1.05607800	-3.98762000	-2.14625800
H	-9.77364700	0.95349000	-3.27031200	C	-1.29272800	-5.06289200	-1.26841900
H	-11.40149900	0.49345100	-1.45961700	C	-1.92455600	-3.82940000	-3.24466800
C	2.25266100	3.69500800	-1.13665100	C	-2.36011000	-5.93349900	-1.47061200
C	2.43388400	4.69943600	-0.16509900	H	-0.61070700	-5.21535300	-0.43815100
C	1.28207800	3.89332800	-2.13995200	C	-3.00000800	-4.69577800	-3.43998700
C	1.65813200	5.86197500	-0.19216600	H	-1.75814800	-3.01430400	-3.94314200
H	3.15951900	4.58305900	0.62752800	C	-3.22541400	-5.75064600	-2.55301100
C	0.50658700	5.05587400	-2.15884200	H	-2.51587100	-6.76080600	-0.78313600
H	1.13126800	3.15884300	-2.92058500	H	-3.66201000	-4.54766600	-4.28990900

H	-4.06180100	-6.42704300	-2.70695200	C	3.92949600	2.08212500	-2.15573700
C	-3.19520400	-2.65909000	1.64056300	C	2.82170000	1.70098000	-2.93837700
C	-2.68435100	-1.15005900	3.90148400	C	4.58711500	3.28961400	-2.46855700
C	-1.94774000	0.14372500	4.37058700	C	2.41634100	2.47658800	-4.02763900
H	-0.95320900	0.25053000	3.90322200	H	2.26383100	0.80682300	-2.71549700
H	-2.54068500	1.05407800	4.14193600	C	4.16712800	4.07072400	-3.54941200
H	-1.79682200	0.15673700	5.47198800	H	5.41541700	3.64238700	-1.86787000
C	-4.12003400	-1.02928300	4.48856600	C	3.08813900	3.66044600	-4.33341900
H	-4.66729800	-1.98544600	4.51793400	H	1.56862800	2.16671900	-4.62510800
H	-4.07467800	-0.70876400	5.55277600	H	4.67865200	4.99676300	-3.77785900
H	-4.72805100	-0.27143400	3.96037000	H	2.76446000	4.26612000	-5.16983600
C	-1.98301400	-2.32553200	4.62551500	C	7.67253600	0.37424400	0.69407500
H	-1.82691000	-2.10120300	5.70299200	C	8.61346500	0.14313000	-0.32674700
H	-2.60331400	-3.24110700	4.61642800	C	8.12849800	0.55075200	2.01426600
H	-0.98708800	-2.53599000	4.18555400	C	9.97893900	0.08782400	-0.03110900
C	-4.50333700	-3.22794700	2.25373000	H	8.29144200	-0.01092800	-1.34912700
H	-4.31202300	-3.73540600	3.21942800	C	9.49515900	0.49509400	2.30399500
H	-5.30160100	-2.48873700	2.40375900	H	7.43037400	0.74852300	2.81820500
H	-4.93009400	-4.01457600	1.59353600	C	10.41939000	0.26346600	1.28269900
C	-2.15988600	-3.82259300	1.73898600	H	10.69591300	-0.09453700	-0.82117600
H	-1.91433400	-4.12078100	2.76808700	H	9.83801500	0.63521500	3.32101500
H	-2.55921900	-4.74325200	1.26103300	H	11.47687400	0.22054100	1.50927900
H	-1.21467300	-3.57600100	1.22319100	C	-2.08080600	3.64181600	1.28919200
C	-3.42535800	-2.48153000	0.11522700	C	-2.26365000	4.70085200	0.37783500
H	-4.28559800	-1.83258300	-0.12593300	C	-1.07573400	3.76168400	2.27070300
H	-2.51549100	-2.06689500	-0.35658600	C	-1.45527900	5.83958100	0.44083400
H	-3.64465600	-3.45226200	-0.37908300	H	-3.01771000	4.64698800	-0.39463500
C	2.68409800	-0.02073500	3.20287900	C	-0.26768500	4.90063200	2.32543400
C	3.17539300	-2.48988400	2.02969100	H	-0.92361100	2.98439400	3.00830900
C	1.89648600	-3.30093900	2.41242400	C	-0.45658500	5.93831300	1.41119100
H	1.01717500	-3.02644100	1.80642100	H	-1.59753300	6.64264500	-0.27062400
H	2.05354100	-4.39073100	2.25595900	H	0.50395900	4.97940800	3.08026800
H	1.63113200	-3.20885000	3.48057000	H	0.17181200	6.81835700	1.45361300
C	3.64427600	-3.07977000	0.67127600	C	-6.57114700	1.51543100	0.62175100
H	2.88685000	-2.90285300	-0.11123200	C	-7.17811900	0.51652500	-0.16283200
H	4.61104500	-2.65110900	0.33887700	C	-7.34107900	2.61896100	1.03454900
H	3.79791800	-4.17923400	0.73656700	C	-8.52230300	0.62405200	-0.53026300
C	4.24803200	-2.89966700	3.07485900	H	-6.60718400	-0.33606400	-0.50937100
H	4.31761100	-4.00878900	3.12636600	C	-8.68632200	2.71979900	0.66682900
H	5.26887200	-2.57923600	2.81907300	H	-6.90807100	3.63947600	1.63526900
H	3.99132400	-2.58552100	4.09972100	C	-9.27591100	1.72440400	-0.11585600
C	1.73858500	-0.69151400	4.22363300	H	-8.97867200	-0.14478100	-1.14023600
H	1.39233300	0.03603200	4.99019600	H	-9.27263500	3.57002300	0.99062600
H	0.84246100	-1.08920600	3.71437100	H	-10.31683600	1.80567200	-0.40095300
H	2.23609500	-1.49964200	4.78942400	C	-2.78564400	0.79318300	-2.18861000
C	3.99922400	0.34598300	3.94497800	C	-3.22883800	-0.46105000	-2.64048000
H	3.77153800	0.82487300	4.92249800	C	-3.66143800	1.89051800	-2.26420400
H	4.64012700	-0.52224900	4.16246500	C	-4.51242200	-0.61569600	-3.15173800
H	4.59419000	1.09000400	3.37538700	H	-2.55634200	-1.30833300	-2.58944900
C	2.01934200	1.34102600	2.83922800	C	-4.95431300	1.72863000	-2.75724800
H	1.93283100	1.99808000	3.73250400	H	-3.34723300	2.86039900	-1.90012500
H	2.61160100	1.89652400	2.08309400	C	-5.38177600	0.47740700	-3.20469600
H	0.99167900	1.19817600	2.44849200	H	-4.83670200	-1.59342500	-3.49589600
C	-3.22885300	0.01549800	1.68214400	H	-5.63105000	2.57795300	-2.77972600
C	-4.60327800	0.17771900	1.40344600	H	-6.39190300	0.35257200	-3.58509400
C	-2.41017700	1.16149600	1.53758300	C	1.06251200	-2.77144700	-2.92673400
C	-5.13674800	1.40849500	0.98988700	C	2.14716300	-1.91075400	-2.63695100
H	-5.28964000	-0.63274200	1.51918200	C	1.04966600	-3.38873100	-4.20454300
C	-2.94227700	2.42735400	1.23770700	C	3.16176000	-1.68899800	-3.55936800
H	-1.35030100	1.08890900	1.72549400	H	2.17847700	-1.43547500	-1.66581100
C	-4.30672300	2.53463000	0.94318700	C	2.05718700	-3.14438200	-5.13052200
H	-4.72756400	3.49620400	0.67985300	H	0.26616700	-4.09383400	-4.45612500
C	3.90687200	-0.18990300	0.94096800	C	3.12372500	-2.29506800	-4.81904200
C	5.29126600	-0.20707400	1.21463700	H	3.99207200	-1.03847600	-3.29505100
C	3.48880700	0.54971900	-0.19558100	H	2.02112400	-3.63879800	-6.09831500
C	6.22205300	0.43133600	0.38211900	H	3.91630400	-2.11732200	-5.54074600
H	5.66946800	-0.69751700	2.08504600				
C	4.40040900	1.23726700	-1.01790000	----			
H	2.44369100	0.63492500	-0.42880100	benzophenone transition state triplet			
C	5.76930900	1.14126300	-0.73456900	----			
H	6.48863800	1.63932400	-1.37249400	Cr	0.13605900	-0.17361300	-0.27175600

O	-0.61637800	0.26537700	-1.84539200	H	1.90571900	-4.46530100	1.78579000
O	1.38624300	-1.42762600	-0.50833500	H	0.88271500	-3.72518700	0.51586300
C	-1.78986500	0.67168100	-2.60525000	H	2.17631300	-4.93221300	0.10922400
C	2.67763500	-2.05050600	-0.73344200	C	4.35036300	-3.56775100	0.75758400
O	0.80101500	0.97151500	1.03710700	H	4.34792300	-4.29660800	1.59786500
O	-1.33096400	-0.19149900	0.85202700	H	4.69718600	-4.12139500	-0.12638500
C	-1.28365600	-0.00857500	2.18548100	H	5.11975400	-2.81907700	1.03726900
C	0.13413600	1.53145100	2.06243700	C	2.78193900	-2.00665400	1.83832200
C	-0.67051100	-1.18262500	2.94793700	H	2.90406400	-2.57746500	2.78504300
C	-0.85474300	-2.45136600	2.37148500	H	3.55449400	-1.21042000	1.83543600
C	-0.09466700	-1.12482700	4.22580200	H	1.78771700	-1.52591200	1.87051300
C	-0.48977000	-3.61342300	3.04766600	C	-2.98263400	-0.14444700	-2.03694200
H	-1.30069000	-2.51829800	1.38792600	C	-4.33025900	0.22064500	-2.24122600
C	0.29201100	-2.28848000	4.89221900	C	-2.74517800	-1.35634100	-1.34490300
H	0.07151100	-0.17589900	4.71350600	C	-5.38933000	-0.51283900	-1.68256400
C	0.09404900	-3.53955200	4.31121800	H	-4.58111200	1.07103300	-2.83904200
H	-0.65127700	-4.57958700	2.57858400	C	-3.79161600	-2.12141800	-0.80908100
H	0.74861900	-2.20760200	5.87512400	H	-1.73592400	-1.72032400	-1.21530800
H	0.38820900	-4.44462400	4.83570700	C	-5.11011500	-1.68022700	-0.96253400
C	-0.50170000	2.88473300	1.74567100	H	-5.92159200	-2.25424600	-0.53189300
C	0.27333500	3.75051500	0.95333900	C	3.73395500	-0.91805200	-0.85940700
C	-1.68603800	3.38589400	2.30222200	C	5.11592800	-1.18051000	-1.00013600
C	-0.13474400	5.05936500	0.70637000	C	3.33267000	0.43859400	-0.90416400
H	1.21126100	3.38779100	0.54647100	C	6.06666100	-0.14833200	-1.05140300
C	-2.09697000	4.69668100	2.04857800	H	5.48319400	-2.18364200	-1.08084600
H	-2.30451800	2.76150800	2.93055900	C	4.27028400	1.47979900	-0.96301600
C	-1.32711500	5.53952000	1.24962100	H	2.28884100	0.70680300	-0.91491300
H	0.48007400	5.70846600	0.08997800	C	5.63394300	1.18091000	-1.00989400
H	-3.02774600	5.05328800	2.48195800	H	6.35697600	1.98756200	-1.04178100
H	-1.64806400	6.55936500	1.05519800	C	3.82700200	2.88752900	-1.00637400
C	-1.90816700	2.27290100	-2.34439300	C	2.92133400	3.31343600	-1.99113800
C	-1.52145000	0.18562400	-4.11845800	C	4.33600300	3.82213800	-0.08809500
C	-1.21759200	-1.33947300	-4.13932800	C	2.53459400	4.65542900	-2.05855700
H	-0.38334200	-1.58193700	-3.46394400	H	2.53256800	2.61066000	-2.71773600
H	-2.10209300	-1.94308000	-3.84898800	C	3.94025600	5.16058000	-0.15389100
H	-0.92699100	-1.68550900	-5.15544000	H	5.03310700	3.51111500	0.68067500
C	-2.72219200	0.36699200	-5.08846200	C	3.04474900	5.57827400	-1.14176200
H	-2.97223400	1.41627000	-5.30091000	H	1.84131600	4.98075900	-2.82319400
H	-2.48045900	-0.07514200	-6.07998700	H	4.33116600	5.87549600	0.55838900
H	-3.62833500	-0.15889900	-4.73017900	H	2.74249800	6.16144400	-0.19412000
C	-0.28514500	0.86924000	-4.75330000	C	7.51440700	-0.46268400	-1.15768600
H	0.02213000	0.35333900	-5.68901000	C	8.34408000	0.27153800	-2.02618700
H	-0.49392200	1.91031500	-5.05670800	C	8.07903400	-1.50053700	-0.39216500
H	0.58491100	0.58460100	-4.06570300	C	9.70622600	-0.02798000	-0.12548600
C	-2.66928200	3.11315400	-3.40516800	H	7.93622900	1.06465900	-2.64030000
H	-2.10522800	3.20392100	-4.35095900	C	9.44186400	-1.79522700	-0.49500600
H	-3.68667300	2.75896100	-3.62152700	H	7.47094300	-2.07218600	0.29729800
H	-2.79189900	4.15920400	-3.04708700	C	10.25461800	-1.06005600	-1.36078200
C	-0.50271600	2.93797100	-2.23069100	H	10.33641000	0.53870700	-2.79872900
H	0.06206400	2.91854100	-3.17585100	H	9.86866400	-2.59241800	0.09984800
H	-0.59248800	4.01410500	-1.96652400	H	11.30933300	-1.29007000	-1.43906000
H	0.11951700	2.46742200	-1.44501300	C	-3.50202800	-3.38027200	-0.08222700
C	-2.59435700	2.55151700	-0.98183300	C	-4.14352400	-3.66372500	1.13735300
H	-3.68143200	2.34803300	-0.99970500	C	-2.56637700	-4.29961400	-0.59257600
H	-2.12775700	1.94144000	-0.19075500	C	-3.85765200	-4.84550600	1.82738400
H	-2.49922400	3.61880300	-0.68934300	H	-4.84885600	-2.96215500	1.56540100
C	2.94172100	-2.92502200	0.59575400	C	-2.28344500	-5.47891700	0.10210000
C	2.49333400	-2.82759900	-2.13944300	H	-2.06428400	-4.11120600	-1.53328100
C	1.12250100	-3.57511700	-2.24609900	C	-2.93186200	-5.75395600	1.30846600
H	0.27465200	-2.99929600	-1.83212200	H	-4.35009500	-5.05435600	2.76820700
H	0.87191000	-3.80389700	-3.30462300	H	-1.56160500	-6.18030600	-0.29592100
H	1.13027300	-4.56222900	-1.75051700	H	-2.70979100	-6.66660800	1.84603200
C	2.51256300	-1.78742400	-3.29738500	C	-6.78976300	-0.05092500	-1.84807900
H	1.82076100	-0.94873100	-3.08256800	C	-7.11217700	1.31117600	-1.69936500
H	3.52908900	-1.36428600	-3.44431200	C	-7.81618400	-0.96599600	-2.14752400
H	2.21795400	-2.24025100	-4.26896900	C	-8.43243500	1.74590900	-1.84884800
C	3.57179700	-3.88268200	-2.47983000	H	-6.34647100	2.03566100	-1.45079500
H	3.38952200	-4.29400500	-3.49717500	C	-9.13475700	-0.52545500	-2.29703500
H	4.59116500	-3.46540900	-2.50958000	H	-7.59623900	-2.01775700	-2.28149700
H	3.52322200	-4.75536400	-1.80144300	C	-9.44266200	0.82882700	-2.14778200
C	1.91082800	-4.06771600	0.74798600	H	-8.67284700	2.79442100	-1.72919300

H	-9.91809700	-1.23464000	-2.53142000	H	-0.60075900	1.65222400	-5.14069800
H	-10.46413100	1.16750200	-2.26330100	H	0.49641100	0.61614100	-4.13693100
C	-2.63503900	0.37351200	2.74942300	C	-2.75495000	2.91976400	-3.48084200
C	-3.72672000	0.53710000	1.88015700	H	-2.22630000	2.95994000	-4.45060900
C	-2.86416200	0.52653400	4.12854400	H	-3.78792300	2.57682500	-3.63456900
C	-4.99221900	0.86085700	2.36326800	H	-2.84703700	3.98160300	-3.16206200
H	-3.57881900	0.38624400	0.82090500	C	-0.56342000	2.78793200	-2.35218500
C	-4.12641200	0.86982400	4.61053000	H	-0.01817900	2.73473600	-3.30780200
H	-2.05724400	0.37516700	4.83523000	H	-0.65370400	3.87217300	-2.12347200
C	-5.19855700	1.04039600	3.73176100	H	0.07645800	2.35093500	-1.56256200
H	-5.81802800	0.97043300	1.66464400	C	-2.62947400	2.41878500	-1.04787000
H	-4.27456700	0.99019700	5.68057600	H	-3.71771100	2.21443700	-1.04945100
H	-6.18351200	1.29815200	4.11158000	H	-2.15619600	1.81315700	-0.25464100
C	0.96869100	1.64760900	3.31517400	H	-2.52683900	3.49080300	-0.77669400
C	2.30764200	1.23368200	3.29105400	C	2.82418600	-2.87033500	0.75213300
C	0.47527900	2.24052800	4.49160100	C	2.28985100	-3.05262800	-1.96456300
C	3.11804100	1.36069200	4.41827900	C	0.88780800	-3.74365000	-1.97659700
H	2.70837100	0.85068200	2.36264300	H	0.06666100	-3.06604400	-1.68698700
C	1.28107500	2.35502600	5.62212000	H	0.64291800	-4.13066600	-2.98959000
H	-0.54369100	2.61008600	4.52576000	H	0.83748200	-4.62973500	-1.32020700
C	2.60588700	1.90896700	5.59449400	C	2.34364100	-2.14765400	-3.23016900
H	4.15461700	1.03668300	4.37236500	H	1.72094300	-1.24087900	-3.09372000
H	0.87683300	2.80585000	6.52483600	H	3.38218200	-1.81587300	-3.44383700
H	3.23485900	2.00697700	6.47523800	H	1.98990700	-2.68069900	-4.13931600
				C	3.31144200	-4.19009200	-2.19710800
				H	3.11074600	-4.68660100	-3.17213500
				H	4.35157200	-3.83120000	-2.25691200
				H	3.21415400	-4.99081700	-1.43880400
				C	1.74866800	-3.93382200	1.08144900
				H	1.78127800	-4.21520300	2.15581900
				H	0.72466100	-3.56809700	0.86349300
				H	1.93834400	-4.87509800	0.53012900
				C	4.20988700	-3.56089000	0.92490700
				H	4.21264800	-4.19297800	1.84014600
				H	4.49668300	-4.22267600	0.09712600
				H	5.02526600	-2.82759700	1.08992000
				C	2.77562500	-1.80696900	1.88400300
				H	2.87260400	-2.27404900	2.88841100
				H	3.60635200	-1.07736600	1.78167000
				H	1.83241700	-1.23862600	1.86527800
				C	-3.02709800	-0.28242600	-2.00255800
				C	-4.37791700	0.04195400	-2.24864400
				C	-2.77630200	-1.41300800	-1.19003200
				C	-5.43042900	-0.64553000	-2.02942000
				H	-4.63401600	0.82221100	-2.93465300
				C	-3.81424600	-2.12334800	-0.56939500
				H	-1.76569600	-1.75149200	-1.02313700
				C	-5.13810900	-1.72058800	-1.77502000
				H	-5.94296200	-2.25290200	-0.28272300
				C	3.59322200	-1.04464500	-0.92093000
				C	4.96749300	-1.34222800	-1.06311100
				C	3.21308200	0.30804500	-1.07005300
				C	5.93451800	-0.33151900	-1.19478000
				H	5.31332300	-2.35658200	-1.07702500
				C	4.16602700	1.32907100	-1.18242400
				H	2.17492300	0.58711900	-1.10831000
				C	5.52427300	1.00605900	-1.22177500
				H	6.25971000	1.79853900	-1.29693400
				C	3.74206300	2.74058100	-1.25364500
				C	2.84805000	3.16251900	-2.25000500
				C	4.23850300	3.67614100	-0.33068100
				C	2.46016900	4.50386700	-2.32468600
				H	2.46520900	2.45600300	-2.97612200
				C	3.84204700	5.01475100	-0.40395800
				H	4.92212700	3.36661000	0.45050800
				C	2.95732800	5.42913200	-1.40307300
				H	1.77412900	4.82617900	-3.09712300
				H	4.22176500	5.73108200	0.31292300
				H	2.65343400	6.46624500	-1.46042200
				C	7.37556300	-0.67524700	-1.30081600
				C	8.20417100	-0.00468600	-2.22032300

benzophenone diolate triplet

Cr	0.10159900	-0.15808200	-0.30753800
O	-0.65079300	0.12838800	-1.88330800
O	1.24057900	-1.48001900	-0.44374400
C	-1.84857500	0.50760300	-2.63094500
C	2.52709900	-2.13991500	-0.65226200
O	0.72867300	1.15752400	0.73448800
O	-1.14168200	-0.29430000	0.96818500
C	-0.92545600	0.28146900	2.26025100
C	0.04761500	1.57194000	1.92380000
C	-0.35679200	-0.85204600	3.17032400
C	-0.75771200	-2.16094300	2.84924300
C	0.38887900	-0.67798500	4.34560800
C	-0.41790400	-3.24511800	3.65489900
H	-1.34334100	-2.32064000	1.95404500
C	0.73901500	-1.76793400	5.14766000
H	0.71332800	0.30126700	4.65959300
C	0.34142700	-3.05791400	4.80945500
H	-0.73807800	-4.24363400	3.37209900
H	1.32864900	-1.59321000	6.04405200
H	0.61383700	-3.90380400	5.43509500
C	-0.60436100	2.95505600	1.60371900
C	0.16857600	3.80849300	0.79242700
C	-1.78173100	3.48219600	2.15115000
C	-0.23432400	5.11012000	0.51030500
H	1.10301900	3.43915400	0.38708100
C	-2.18662300	4.79161100	1.86719500
H	-2.40439800	2.89528100	2.80630200
C	-1.42308400	5.61192200	1.04349200
H	0.38428700	5.73733400	-0.12531500
H	-3.11205900	5.16063100	2.30207300
H	-1.74128400	6.62783100	0.82477700
C	-1.96656400	2.11259500	-2.41576900
C	-1.61361600	-0.03540700	-4.12712900
C	-1.31812300	-1.56135100	-4.09264900
H	-0.45649300	-1.77885700	-3.44647300
H	-2.18920200	-2.14515400	-3.72930200
H	-1.07554100	-1.95341600	-5.10468900
C	-2.83053900	0.10862000	-5.08364400
H	-3.13182000	1.14658100	-5.27938700
H	-2.58108800	-0.31448500	-6.08153500
H	-3.70956000	-0.46130700	-4.72370100
C	-0.38742600	0.62050900	-4.80810600
H	-0.10055300	0.07029900	-5.73069200

C	7.93531400	-1.67627200	-0.48434200	C	-1.268382	4.181975	-1.778160
C	9.56020000	-0.33063200	-2.31995700	H	-1.646972	2.327681	-2.817847
H	7.79977500	0.75879200	-2.87310600	H	-0.722395	5.855093	-0.526505
C	9.29207100	-1.99761700	-0.58776400	H	-1.750832	4.798205	-2.531144
H	7.32901600	-2.19772400	0.24503000	C	2.949799	-3.025402	1.043910
C	10.10364600	-1.32591800	-1.50467500	C	3.247668	-2.957968	-1.723637
H	10.18942300	0.18695400	-3.03249200	C	2.847889	-2.061025	-2.935926
H	9.71518300	-2.76599900	0.04634300	H	1.762882	-1.822447	-2.932468
H	11.15365100	-1.57646500	-1.58324300	H	3.417050	-1.108625	-2.947861
C	-3.50829100	-3.27275200	0.31471900	H	3.065524	-2.571162	-3.900023
C	-4.14382300	-3.40071600	1.56329500	C	4.753127	-3.283809	-1.924138
C	-2.56390100	-4.24053500	-0.07416900	H	5.199311	-3.860658	-1.106232
C	-3.84314300	-4.47869400	2.40110700	H	4.893565	-3.892735	-2.848883
H	-4.85650500	-2.65705500	1.89799000	H	5.354098	-2.364443	-2.082662
C	-2.26490300	-5.31479400	0.76829900	C	2.446349	-4.269155	-1.901001
H	-2.07067300	-4.17395700	-1.03524400	H	2.569856	-4.673378	-2.929581
C	-2.90818800	-5.43704700	2.00216800	H	2.792176	-5.072139	-1.227870
H	-4.33122400	-4.56794700	3.36291100	H	1.363682	-4.092077	-1.755472
H	-1.53621700	-6.05440600	0.46260800	C	4.113088	-4.037126	1.223242
H	-2.67479900	-6.26911400	2.65366000	H	4.065722	-4.871335	0.502646
C	-6.83729500	-0.23132200	-1.85197200	H	5.113110	-3.580798	1.198435
C	-7.18450200	1.13283300	-1.87157800	H	4.048525	-4.515626	2.225229
C	-7.84516400	-1.19401800	-2.04791900	C	1.643577	-3.845383	1.271906
C	-8.51030900	1.52244500	-2.08364700	H	1.473207	-4.616464	0.503455
H	-6.43406700	1.89607300	-1.70622200	H	1.673752	-4.384207	2.244459
C	-9.16935700	-0.79855600	-2.26044300	H	0.755176	-3.189479	1.315442
H	-7.60634500	-2.25016000	-2.05321700	C	3.019418	-2.044644	2.249042
C	-9.50168100	0.55799600	-2.27819600	H	4.008980	-1.551616	2.326923
H	-8.76966400	2.57322500	-2.09364000	H	2.239001	-1.261407	2.165181
H	-9.93804500	-1.54482500	-2.41443400	H	2.861976	-2.574469	3.214181
H	-10.52744100	0.86179600	-2.44242300	C	-2.518373	-2.725621	-1.277343
C	-2.32434400	0.57282500	2.85271200	C	-3.255260	-3.366561	1.334449
C	-3.46827500	0.48417300	2.05115600	C	-2.096045	-4.270302	1.858448
C	-2.49547800	0.85922100	4.21660600	H	-1.312711	-3.675643	2.372437
C	-4.74027800	0.70213300	2.58216700	H	-2.471393	-4.996592	2.612608
H	-3.36301600	0.23432000	1.00638900	H	-1.623844	-4.877359	1.069711
C	-3.76379700	1.09313200	4.74589200	C	-3.798633	-2.650104	2.606371
H	-1.63568700	0.89665600	4.87651200	H	-3.063790	-1.905855	2.982746
C	-4.89587800	1.01663300	3.93093600	H	-4.759550	-2.131300	2.408141
H	-5.60889400	0.62259200	1.93304800	H	-3.999125	-3.372965	3.427548
H	-3.86731200	1.32130800	5.80361200	C	-4.369961	-4.328254	0.857122
H	-5.88485800	1.18826500	4.34736500	H	-4.684906	-4.993655	1.690797
C	1.13473300	1.92449900	2.96263500	H	-5.287244	-3.803543	0.544694
C	2.47897900	1.63779700	2.70601800	H	-4.020177	-5.006917	0.058237
C	0.81644400	2.62868900	4.13525400	C	-1.604795	-3.968786	-1.378779
C	3.47547100	1.99814800	3.61566200	H	-1.253421	-4.122607	-2.422721
H	2.74180200	1.15459300	1.77495100	H	-0.704007	-3.848191	-0.745862
C	1.80789100	2.97725700	5.05019700	H	-2.137655	-4.896731	-1.099846
H	-0.21286000	2.90985400	4.33432200	C	-3.795596	-3.012434	-2.116115
C	3.14519300	2.65862900	4.79735700	H	-3.520085	-3.468345	-3.092414
H	4.51305100	1.76346500	3.39143200	H	-4.498070	-3.712800	-1.642795
H	1.53657600	3.51348100	5.95600500	H	-4.335015	-2.078077	-2.375288
H	3.91910600	2.93947000	5.50672200	C	-1.780572	-1.588648	-2.042824
----				H	-1.650272	-1.845911	-3.117155
mono-benzaldehyde triplet				H	-2.348418	-0.635365	-2.001271
----				H	-0.767112	-1.413126	-1.636684
Cr	0.146900	-1.104858	0.449152	C	3.734176	-0.883912	-0.296403
O	1.520928	-1.787971	-0.495985	C	5.103402	-0.881510	0.045976
O	-1.437891	-1.897944	0.732170	C	3.157348	0.358342	-0.660069
C	2.896822	-2.191741	-0.352454	C	5.856070	0.302404	0.087389
C	-2.743681	-2.268782	0.252550	H	5.605951	-1.796222	0.278557
O	0.564846	0.511982	1.275008	C	3.904330	1.546990	-0.655144
C	0.532622	1.794974	1.237248	H	2.127897	0.413163	-0.985095
C	-0.031718	2.583902	0.180964	C	5.245087	1.513349	-0.256154
C	-0.596187	2.002717	-0.976903	H	5.832808	2.423469	-0.275388
C	-0.077233	3.991149	0.317108	C	-3.634688	-0.997596	0.300013
C	-1.211952	2.792732	-1.937556	C	-4.999742	-1.026565	-0.060133
H	-0.541578	0.928080	-1.111007	C	-3.120123	0.228742	0.786203
C	-0.689723	4.776132	-0.649398	C	-5.813585	0.113139	0.027274
H	0.361561	4.452553	1.198666	H	-5.452330	-1.928093	-0.421575
				C	-3.927297	1.372598	0.905733

H	-2.088453	0.308397	1.090414	H	-3.707200	-0.965295	5.128699
C	-5.268456	1.307766	0.509759	C	-2.240399	2.387342	-1.707154
H	-5.905890	2.175743	0.627941	C	-2.002851	0.317806	-3.557845
C	-3.386861	2.624571	1.493872	C	-1.650544	-1.200275	-3.581941
C	-2.558807	2.580052	2.631447	H	-0.678257	-1.400529	-3.089437
C	-3.723991	3.876575	0.946016	H	-2.429630	-1.809526	-3.077658
C	-2.079572	3.761572	3.204885	H	-1.567136	-1.576592	-4.625274
H	-2.296216	1.633703	3.087356	C	-3.271084	0.458123	-4.444584
C	-3.246891	5.055265	1.527195	H	-3.712286	1.465306	-4.436581
H	-4.345168	3.942781	0.061622	H	-3.025611	0.234616	-5.505911
C	-2.424939	4.997988	2.654864	H	-4.052226	-0.276814	-4.160786
H	-1.442315	3.718189	4.078534	C	-0.835827	1.031929	-4.282719
H	-3.506767	6.013523	1.096532	H	-0.598529	0.527106	-5.244790
H	-2.051591	5.911344	3.099334	H	-1.092565	2.073220	-4.550740
C	-7.244507	0.048261	-0.364510	H	0.091155	1.012635	-3.671173
C	-7.829137	1.091506	-1.106864	C	-3.127737	3.240796	-2.647068
C	-8.038038	-1.055952	0.000596	H	-2.734245	3.271547	-3.679079
C	-9.176032	1.028334	-1.476776	H	-4.185446	2.935949	-2.650100
H	-7.240463	1.946833	-1.414481	H	-3.135819	4.298949	-2.304423
C	-9.384532	-1.113447	-0.371524	C	-0.835613	3.067462	-1.721996
H	-7.622235	-1.865364	0.587776	H	-0.376498	3.089345	-2.723765
C	-9.952875	-0.072867	-1.109755	H	-0.905333	4.130815	-1.403440
H	-9.616907	1.832762	-2.051269	H	-0.128095	2.584028	-1.022087
H	-9.988698	-1.964227	-0.083989	C	-2.779149	2.602473	-0.262765
H	-10.995379	-0.119571	-1.396913	H	-3.861577	2.369329	-0.190176
C	3.306475	2.817395	-1.131220	H	-2.235293	1.959671	0.459448
C	2.556609	2.848514	-2.321325	H	-2.664096	3.658434	0.066323
C	3.521541	4.016368	-0.427565	C	2.629716	-2.720048	1.615620
C	2.046075	4.057337	-2.803031	C	1.988313	-3.144968	-1.065725
H	2.386061	1.942771	-2.889975	C	0.493955	-3.592303	-1.042091
C	3.003356	5.221746	-0.910566	H	-0.199171	-2.728712	-1.106979
H	4.084979	4.018352	0.497225	H	0.259473	-4.242446	-1.913466
C	2.271810	5.243228	-2.100329	H	0.239126	-4.184624	-0.148244
H	1.473672	4.074359	-3.721377	C	2.168947	-2.421707	-2.432296
H	3.169474	6.139825	-0.362159	H	1.653440	-1.437398	-2.427170
H	1.870919	6.177060	-2.472416	H	3.240634	-2.255012	-2.667928
C	7.292227	0.269465	0.463520	H	1.752757	-3.020867	-3.271707
C	7.828330	1.250993	1.318148	C	2.818321	-4.449045	-1.134648
C	8.139429	-0.741520	-0.028949	H	2.533192	-5.035972	-2.035371
C	9.180304	1.218376	1.673194	H	3.900314	-4.270626	-1.237378
H	7.198375	2.032857	1.723833	H	2.614915	-5.114461	-0.275154
C	9.490731	-0.768775	0.328940	C	1.482340	-3.638989	2.104923
H	7.761563	-1.499510	-0.703756	H	1.577492	-3.848658	3.192739
C	10.010581	0.209599	1.179423	H	0.488693	-3.167086	1.953997
H	9.583751	1.974458	2.334321	H	1.509344	-4.626237	1.606926
H	10.136183	-1.547382	-0.056657	C	3.965960	-3.493521	1.801270
H	11.056918	0.186435	1.455284	H	3.991664	-3.979058	2.801407
H	0.934284	2.311822	2.113643	H	4.129239	-4.296735	1.069903
----				H	4.841894	-2.813566	1.786667
mono-benzophenone				C	2.703649	-1.539447	2.631801
----				H	2.882734	-1.909896	3.665099
Cr	0.140510	0.098249	-0.011640	H	3.535003	-0.844779	2.387666
O	-0.936573	0.376653	-1.408561	H	1.767203	-0.950362	2.655831
O	1.138970	-1.359712	0.311777	C	-3.321419	0.019057	-1.359297
C	-2.156225	0.797141	-2.029685	C	-4.671802	0.276932	-1.678130
C	2.341677	-2.126611	0.146525	C	-3.063382	-0.979585	-0.388006
O	0.311903	1.461596	1.235918	C	-5.724505	-0.417142	-1.064005
C	-0.066566	1.893740	2.395093	H	-4.928285	0.995510	-2.429914
C	-1.065679	1.131897	3.153301	C	-4.106289	-1.699377	0.222985
C	-1.980521	1.756496	4.028148	H	-2.049500	-1.208496	-0.091732
C	-1.162202	-0.265596	2.980288	C	-5.432301	-1.405748	-0.118336
C	-2.930123	1.009086	4.719017	H	-6.241385	-1.953669	0.348758
H	-1.963627	2.835624	4.138265	C	3.488597	-1.157253	-0.251445
C	-2.084769	-1.009789	3.705661	C	4.795727	-1.612950	-0.529497
H	-0.484560	-0.781777	2.308676	C	3.250120	0.231176	-0.371908
C	-2.978415	-0.380235	4.574725	C	5.831047	-0.728214	-0.873861
H	-3.636403	1.513780	5.372768	H	5.029682	-2.658396	-0.488607
H	-2.093030	-2.089224	3.596890	C	4.268289	1.127440	-0.726584
				H	2.276140	0.642459	-0.177850
				C	5.558284	0.642382	-0.965581
				H	6.349539	1.334112	-1.228824

C	3.977380	2.574889	-0.850698	H	2.225397	5.826072	1.574775
C	2.851036	3.013975	-1.569512	H	1.353066	4.888529	5.681573
C	4.823227	3.527221	-0.254867	H	2.350982	6.415231	3.988571
C	2.578312	4.380003	-1.689392				
H	2.194222	2.300264	-2.051338	----			
C	4.543006	4.891966	-0.373106	benzaldehyde			
H	5.690312	3.214112	0.313408	----			
C	3.422694	5.317896	-1.090963	C	1.992201	0.468751	0.000049
H	1.713063	4.712200	-2.247793	H	2.274032	1.545722	0.000071
H	5.193699	5.619773	0.094038	O	2.847537	-0.395876	-0.000062
H	3.207555	6.374702	-1.181198	C	0.533956	0.214513	0.000025
C	7.199149	-1.240553	-1.140771	C	-0.361112	1.292134	0.000001
C	7.952370	-0.741162	-2.220040	C	0.045248	-1.101093	0.000028
C	7.763387	-2.234504	-0.318661	C	-1.735949	1.060572	-0.000018
C	9.239495	-1.226991	-2.469684	H	0.024976	2.309563	-0.000002
H	7.539546	0.011444	-2.880086	C	-1.326223	-1.331252	0.000006
C	9.051145	-2.716100	-0.572623	H	0.759096	-1.919241	0.000047
H	7.215919	-2.626534	0.529317	C	-2.216809	-0.250815	-0.000016
C	9.788385	-2.213205	-1.646975	H	-2.430299	1.896107	-0.000035
H	9.810474	-0.840632	-3.304088	H	-1.707793	-2.348582	0.000007
H	9.478965	-3.477723	0.066458	H	-3.288190	-0.433416	-0.000033
H	10.784996	-2.587660	-1.841930				
C	-3.812435	-2.772903	1.207010	----			
C	-4.597065	-2.919999	2.367263	benzophenone			
C	-2.752862	-3.671020	0.985629	----			
C	-4.317995	-3.936544	3.286292	C	0.000025	1.079997	0.000011
H	-5.409417	-2.235404	2.575889	O	0.000091	2.306319	0.000159
C	-2.472784	-4.680981	1.910277	C	-1.303847	0.337002	0.024002
H	-2.158847	-3.605334	0.085881	C	-1.454514	-0.925754	0.617699
C	-3.254868	-4.814026	3.059715	C	-2.433877	0.983257	-0.502574
H	-4.920200	-4.037092	4.179912	C	-2.709248	-1.534120	0.670776
H	-1.652785	-5.364606	1.731539	H	-0.597020	-1.421159	1.061568
H	-3.037367	-5.596899	3.774600	C	-3.680688	0.366694	-0.466949
C	-7.133030	-0.111708	-1.421937	H	-2.309664	1.971347	-0.933789
C	-7.556092	1.221858	-1.579042	C	-3.820974	-0.894508	0.120641
C	-8.065561	-1.148996	-1.611360	H	-2.818015	-2.505822	1.144801
C	-8.881971	1.508481	-1.917569	H	-4.546277	0.869214	-0.890035
H	-6.865738	2.041946	-1.424378	H	-4.796045	-1.373280	0.155016
C	-9.390135	-0.856451	-1.950462	C	1.303849	0.336974	-0.023979
H	-7.766343	-2.185131	-1.514674	C	1.454428	-0.925849	-0.617548
C	-9.798021	0.470632	-2.103230	C	2.433935	0.983284	0.502404
H	-9.200005	2.536607	-2.033001	C	2.709150	-1.534239	-0.670674
H	-10.100094	-1.659939	-2.098400	H	0.596880	-1.421290	-1.061275
H	-10.823873	0.694728	-2.365648	C	3.680729	0.366696	0.466739
C	0.554694	3.135388	2.859857	H	2.309779	1.971438	0.933499
C	1.152667	3.998368	1.914394	C	3.820937	-0.894581	-0.120716
C	0.643434	3.478909	4.226108	H	2.817854	-2.505997	-1.144596
C	1.784652	5.167746	2.318126	H	4.546367	0.869255	0.889679
H	1.101876	3.735366	0.864458	H	4.795996	-1.373374	-0.155126
C	1.285561	4.648265	4.623847				
H	0.238837	2.809186	4.977214				
C	1.853232	5.501885	3.674665				

Table S4. Harmonic frequencies (cm⁻¹) for each optimized structure.

----				142.7760	147.5554	152.9367
bis-benzaldehyde singlet				162.8440	168.2937	177.9599
----				199.7787	207.6601	212.4267
11.3092	14.2836	16.0915		213.5189	224.4954	230.6585
23.3849	24.9553	31.7808		241.9746	248.9901	257.8477
36.3981	39.4439	44.8525		259.1710	261.4374	276.7600
48.3129	52.0423	55.6160		295.7445	297.7586	304.5233
56.2023	57.3338	62.2650		306.7633	314.0826	323.3338
67.4013	72.3353	76.2365		331.7658	337.4709	344.3776
81.5829	83.6720	89.8064		351.5830	355.1082	363.0171
92.0460	97.0097	105.7343		371.4461	379.6843	382.4777
108.4496	115.1575	121.6214		386.3005	391.8905	395.9547
125.7157	131.5021	134.7510		398.2858	402.6725	414.3592

119.0862	123.7488	130.3038	1256.0163	1263.1482	1264.3900
131.4158	136.2833	139.7898	1289.0610	1289.6597	1297.8355
142.6761	160.1677	165.1346	1301.4632	1302.0188	1343.1459
173.5037	195.4755	205.0183	1346.6731	1363.5178	1372.6058
208.9379	212.3880	216.3883	1373.7177	1374.0344	1376.3092
227.4514	238.4918	244.0194	1380.2571	1383.8713	1401.3331
249.0425	258.0894	262.3216	1401.9002	1402.0057	1402.3574
279.1383	284.6833	290.5365	1405.4005	1406.3534	1409.3756
298.8298	309.1725	318.3100	1410.4090	1416.6467	1419.3994
323.8908	337.4395	341.4098	1429.2599	1431.0977	1458.4218
348.5649	356.5886	358.0485	1461.8671	1465.0555	1476.8772
362.8952	363.5869	381.8092	1477.4622	1478.9892	1481.3744
386.9691	388.9000	395.9176	1484.3823	1484.5436	1494.6670
396.8926	410.1563	413.0888	1497.1344	1504.4564	1506.6373
414.3866	419.4185	421.7240	1509.4617	1520.0327	1521.4847
424.4838	425.2758	427.6064	1525.8237	1528.9896	1532.4333
427.7209	432.3732	436.3502	1534.3041	1536.1433	1537.5351
437.6776	441.2783	445.3245	1539.3462	1543.6634	1545.8195
448.0990	458.0538	459.4479	1546.0994	1554.6759	1559.5564
462.7941	470.8094	475.7070	1560.8948	1569.8019	1575.3953
477.9370	478.8416	483.6970	1576.5342	1587.7315	1593.9725
485.8382	493.3614	503.4857	1600.0486	1605.4034	1606.6566
506.5696	511.0341	517.4839	1611.0536	1620.4607	1621.1162
520.7656	527.7268	543.9143	1626.2013	1627.0906	1643.2973
550.3993	550.8167	573.5401	1643.6322	1643.8563	1645.5336
575.2507	582.5527	589.2903	1664.7211	1666.0504	1687.3119
598.4552	604.3235	606.6954	1687.9842	1698.0393	1702.8623
611.7304	616.8990	626.0470	1707.4663	1709.5520	1714.0237
628.9140	629.2162	632.7761	1716.4894	1727.0413	1727.9981
634.8994	665.4200	666.1735	1730.8599	1731.1758	1745.9916
670.7416	674.5304	675.5816	1748.5710	1755.6474	1758.3952
680.3193	689.8536	692.5756	1760.6508	1765.2642	1768.8537
693.4034	694.5610	704.3026	1770.6437	1795.2788	1801.4603
708.4786	729.3552	735.3702	1824.0713	1825.1533	1828.3201
753.3149	759.1159	760.3671	1830.3420	1856.3836	1856.9895
762.0059	767.8971	768.1510	1857.5629	1861.0835	1899.9216
778.5607	780.5197	786.8676	1900.9129	1904.0113	1905.5187
795.1248	804.8433	808.5482	1915.9201	1918.4297	1952.2313
812.6894	814.2583	829.8023	1952.8642	1972.4155	1974.4260
831.0113	837.4132	837.8227	2047.6918	2049.1450	2061.1418
845.1815	847.7656	848.8707	2064.8052	2839.5425	2844.6615
849.9825	853.2066	858.9876	2845.9511	2846.3494	2846.5366
861.2466	878.7444	878.9236	2850.0667	2853.0426	2853.6994
879.7482	879.8013	898.8157	2855.2955	2858.4505	2861.7214
902.8282	904.6422	922.8674	2863.7405	2938.2429	2938.8542
933.6865	943.6017	944.9652	2939.9368	2941.6197	2943.4768
964.7134	965.2795	969.5514	2944.1821	2944.5352	2946.4799
970.1167	993.3858	993.9101	2947.8294	2948.5220	2950.5667
996.2236	996.8670	999.0433	2953.7849	2955.6072	2956.2145
999.6029	1006.8945	1007.8162	2957.4477	2958.6406	2961.9938
1008.6002	1010.4303	1028.6023	2964.3754	2969.8482	2970.6887
1029.5268	1035.4881	1037.3235	2978.1758	2978.7716	2986.1324
1043.2441	1044.1037	1046.5568	2987.3286	3033.5482	3033.5534
1046.6349	1049.2123	1057.5783	3033.6355	3034.6588	3034.7569
1059.4339	1059.9254	1065.8653	3034.8009	3034.8446	3035.5350
1074.1281	1077.9105	1081.8840	3035.6560	3035.9033	3036.6258
1085.2387	1091.9987	1097.3676	3036.6484	3036.7399	3037.6453
1102.6218	1102.9282	1104.9033	3038.3313	3038.3552	3038.3667
1105.4158	1106.0757	1107.7972	3038.9306	3038.9617	3038.9841
1113.6888	1114.2106	1125.9759	3043.1205	3048.7705	3050.7164
1138.4005	1141.3273	1142.2725	3060.5519	3086.2970	3101.0508
1142.4661	1143.0744	1144.1458	3140.0133	3151.5694	3181.0729
1146.2568	1146.7794	1149.5724	3183.1910	3189.6276	3190.9719
1152.0295	1156.8879	1169.3142	3200.0918	3200.6272	3212.1686
1170.2614	1175.2867	1177.8152	3213.2041	3223.7378	3228.9809
1178.7095	1179.0098	1181.9104			
1182.2408	1185.4600	1187.3166			
1189.1218	1190.6961	1191.0984			
1195.4426	1195.6678	1196.9188			
1202.5606	1206.6640	1216.2355			
1223.7868	1226.3812	1243.3992			

			benzaldehyde transition state triplet		

			-436.2680	12.1154	12.7411
			14.7386	25.4056	36.3737

37.7520	40.6055	48.3995	1173.6291	1174.8496	1176.5846
50.0148	55.5644	56.0405	1177.0463	1178.1674	1180.2960
56.4628	60.4043	64.2602	1181.6598	1183.9118	1186.7727
71.3306	72.7463	80.1773	1192.0246	1192.4055	1192.4988
81.4153	82.2666	87.9273	1194.7700	1201.2524	1203.5247
92.1212	94.8474	100.4851	1205.3750	1207.2262	1214.8673
103.9484	110.3886	118.4150	1221.0468	1223.0462	1226.2964
121.4972	128.5679	129.9805	1231.8104	1234.3577	1265.2917
137.6778	145.4782	149.2033	1271.9639	1286.7617	1292.2097
154.2674	165.1716	176.2551	1293.8690	1299.8164	1301.1078
188.3792	202.2966	211.0082	1337.7231	1341.7508	1366.9019
219.1829	235.7388	236.5740	1368.8365	1372.3958	1372.5270
238.7742	242.5968	246.6225	1380.4520	1381.0755	1401.0667
255.3561	258.2923	258.4883	1401.2747	1401.9384	1401.9452
282.4700	293.4740	295.7254	1405.4146	1406.7060	1407.1733
315.0830	321.2921	322.1749	1412.8458	1418.6323	1421.8278
331.4291	336.9497	343.9292	1427.8183	1429.3975	1432.7565
348.1079	361.7094	378.5345	1441.6965	1458.9164	1459.4289
386.8776	390.8963	395.8804	1474.1485	1477.7977	1480.4369
404.6316	407.8658	410.5264	1483.1835	1489.1537	1493.5761
414.8945	424.5985	426.0960	1502.6662	1506.7862	1507.1263
426.8112	429.0175	429.4507	1507.9881	1510.6796	1516.3120
431.5708	433.3167	434.2544	1517.9156	1525.7588	1530.8715
438.7920	440.4937	448.0434	1540.4660	1541.0168	1541.3086
449.6261	454.2967	456.1554	1541.7803	1544.5958	1548.3334
459.1596	465.3226	473.0256	1549.3425	1555.4736	1555.8312
476.6312	481.5449	486.4350	1565.4743	1572.2255	1575.5721
488.8970	494.4688	496.3999	1580.2555	1584.2689	1595.8507
508.9450	513.9180	518.6470	1596.1395	1598.6672	1603.4075
524.9759	530.3422	542.2656	1614.2685	1624.8599	1629.6895
548.6397	550.5726	556.5432	1638.6438	1639.1557	1640.6565
564.2597	569.9439	577.1692	1642.6033	1656.3525	1657.5897
587.3879	590.0503	593.4188	1661.8243	1666.5840	1685.4413
596.4095	600.2725	610.3978	1688.1100	1694.5837	1701.9899
614.5413	617.7420	624.4244	1704.6582	1711.4914	1712.3109
625.6877	632.9682	634.0683	1717.6864	1721.2642	1728.6422
643.2787	666.0795	667.5940	1728.7867	1732.9439	1740.0109
669.7196	672.2554	675.0896	1744.9287	1750.1139	1750.6074
679.1890	690.0582	692.4162	1764.2622	1764.7819	1766.3167
708.7006	711.4462	718.0133	1773.0329	1789.3214	1799.4643
718.9952	726.2763	738.5300	1823.2240	1823.5301	1827.8382
763.3817	767.6325	767.8114	1828.0946	1853.8238	1854.8825
769.9021	777.1902	779.4088	1856.9469	1857.2460	1897.9919
780.3905	782.1324	783.0608	1898.4424	1902.7509	1903.0832
802.8675	812.2188	812.3475	1914.3699	1915.8338	1951.4082
813.5820	817.3993	829.8295	1952.2671	1972.0335	1973.4172
830.4284	837.9741	838.4686	2046.1472	2050.4620	2058.5862
852.9758	855.4247	859.0775	2064.8216	2840.1355	2840.7140
862.3760	871.0849	875.1017	2843.8271	2844.8289	2848.4408
879.5966	879.7904	879.8662	2850.1234	2852.4656	2855.3574
883.4772	903.2656	904.9422	2859.3940	2859.7295	2861.4833
942.2384	943.4578	944.7536	2869.6276	2937.4205	2939.1006
948.0940	960.3819	962.1626	2939.2534	2942.2217	2942.5101
983.1093	986.0621	994.0735	2943.2524	2945.0337	2946.0176
995.0663	997.0937	999.6720	2947.2429	2947.3523	2948.3944
1000.6855	1005.2211	1007.3166	2949.8818	2950.4719	2953.9507
1009.0348	1011.5855	1018.5965	2955.3990	2958.7673	2968.2776
1019.8992	1024.3473	1024.5080	2971.4907	2976.5453	2979.4120
1028.3974	1029.2948	1040.6975	2983.1953	2988.3501	2995.0949
1042.2447	1050.4053	1053.2069	3007.9856	3033.5700	3033.6382
1054.2957	1054.9920	1057.4244	3033.7715	3033.9731	3034.7639
1062.3351	1066.5935	1076.0531	3034.7767	3034.9314	3035.0257
1080.4901	1081.2533	1081.5401	3035.7878	3035.9436	3036.6672
1097.4857	1099.4247	1103.1760	3036.7446	3036.9787	3037.2669
1103.3585	1104.6231	1106.2626	3038.3337	3038.3631	3038.4135
1107.3457	1107.8809	1110.7271	3038.5347	3038.9568	3038.9977
1111.4366	1116.2539	1133.8039	3039.3186	3039.8448	3044.1875
1141.9383	1142.0714	1142.2588	3045.4346	3080.2504	3111.4879
1143.4517	1143.8730	1145.3632	3115.8436	3125.2673	3184.4846
1145.9693	1149.0473	1149.5865	3185.7003	3194.2422	3195.7202
1150.1487	1161.5869	1169.7858	3205.6722	3208.0996	3214.4640

3221.2883 3244.9259 3250.4152

benzaldehyde diolate triplet

8.2358	9.3089	13.0505
23.7411	29.9351	34.3303
35.8592	40.5905	46.9615
50.8642	52.6479	56.0314
56.7809	63.4333	68.7175
71.5876	73.6204	77.2177
80.8984	82.5402	90.1415
93.4314	97.4209	107.0154
109.7709	117.2333	128.4661
132.6347	134.2769	144.9001
148.5154	159.5130	167.0295
172.6863	182.6455	190.9697
209.5264	211.4029	218.7586
232.3220	234.9435	237.0814
242.4754	257.9476	259.5647
260.4491	263.2785	281.4179
295.1266	305.2532	314.2816
319.5197	325.2909	343.8584
346.5513	350.2022	357.2686
373.6503	378.7924	384.8460
392.6589	398.4780	403.8361
406.9957	413.1592	417.6897
419.6551	420.9261	424.5322
426.2462	427.7227	430.5784
432.6889	435.1790	435.9289
438.5228	444.2314	447.0679
452.8998	454.4382	461.1899
468.2220	470.7407	476.2112
485.1085	492.0663	495.3654
500.1319	505.0392	507.0153
517.0767	523.0716	525.0518
538.8734	549.7568	552.1476
556.5548	559.7322	570.1609
576.2265	588.0838	593.1113
601.3460	601.9724	609.1599
613.8062	621.6615	626.4900
627.2249	629.4413	634.7807
637.4113	638.0581	651.3168
665.7099	667.3694	673.1382
676.4440	687.3385	689.6954
692.9322	708.1738	714.1995
714.5192	722.3950	727.8159
734.3019	747.7388	762.9588
764.0915	767.0688	768.1176
769.2906	778.8732	783.7915
784.3157	790.6711	803.0943
811.9662	812.7674	820.1703
822.5174	831.4946	832.4068
837.1283	840.1544	857.2215
863.0732	865.6286	866.3922
869.3042	879.0681	879.6873
879.8468	883.6932	890.5568
900.5757	911.2656	930.6213
942.1823	943.5019	944.6730
959.0472	966.5090	970.6782
978.1519	993.5460	994.3190
995.9587	996.2214	997.5571
999.9196	1004.9859	1005.9625
1007.3779	1017.8695	1018.9281
1019.9521	1027.1025	1030.1557
1036.4919	1041.2724	1042.5511
1050.8767	1054.1191	1055.1953
1059.8544	1060.4134	1062.8454
1067.7354	1076.0474	1077.6492
1078.5221	1080.3175	1081.2613
1092.9001	1096.1283	1099.2819

1103.3090	1104.3474	1106.0944
1107.5751	1109.5227	1111.4205
1118.1963	1124.0585	1129.8499
1140.2322	1142.1971	1142.2615
1143.0809	1144.6657	1145.7902
1146.7231	1146.8537	1150.0902
1150.2044	1161.5120	1162.7953
1172.7416	1175.0733	1176.1492
1177.7168	1179.4312	1182.0616
1182.6481	1184.9091	1186.3534
1191.3545	1192.0067	1194.1178
1195.1781	1198.0653	1207.7444
1210.7362	1218.5035	1218.9482
1224.7635	1226.0724	1228.0048
1229.7804	1231.2600	1270.5532
1283.5065	1288.7779	1290.6618
1298.0180	1299.1800	1328.6225
1333.3425	1364.8477	1366.4765
1372.0664	1372.4625	1372.8037
1379.7733	1380.2048	1387.7969
1401.6885	1401.7868	1402.2491
1402.3324	1406.4343	1407.1905
1411.4290	1414.5008	1417.3182
1420.0459	1421.1816	1428.9432
1430.0946	1453.1899	1461.3505
1472.2733	1475.0999	1479.5363
1488.4028	1495.5184	1496.7464
1498.4526	1499.3837	1503.8517
1506.8687	1511.6646	1514.9094
1518.6118	1523.2820	1527.6356
1542.6004	1543.7295	1545.0440
1546.7017	1547.9971	1550.6665
1552.0358	1553.6801	1557.3105
1563.5883	1569.9865	1578.1370
1580.2803	1583.7184	1594.6436
1599.3712	1600.1331	1603.3828
1618.8873	1628.1462	1629.8575
1637.1666	1642.4058	1643.7435
1644.5106	1662.6618	1664.2373
1665.9560	1668.6450	1685.1349
1688.3355	1693.5024	1704.7771
1708.3850	1713.5394	1715.4583
1720.1895	1722.4125	1727.4060
1730.7882	1733.9127	1742.6790
1743.4221	1751.1753	1753.9104
1763.9090	1764.6613	1765.8993
1771.4656	1789.2427	1799.6490
1823.3577	1824.1775	1828.1254
1828.4716	1852.7027	1856.7565
1856.9965	1857.8554	1896.1376
1899.7619	1902.3795	1904.1459
1911.8317	1913.3663	1950.0976
1951.3236	1970.4308	1972.1228
2046.0746	2047.0106	2052.0250
2059.8363	2840.0485	2840.8525
2847.9209	2848.9125	2850.2012
2851.5778	2853.8066	2855.1644
2856.4157	2857.1356	2862.5894
2870.7093	2937.2775	2939.1339
2940.2031	2941.4606	2943.8562
2944.1217	2945.2562	2946.0868
2947.1587	2948.4505	2948.8054
2949.3997	2955.1970	2958.1039
2961.4629	2963.9854	2968.3705
2971.6357	2972.3666	2978.7974
2980.4652	2982.7161	2992.9127
3005.7383	3014.7810	3033.5448
3033.5824	3033.5946	3033.6732
3034.7151	3034.7597	3034.7752
3035.2404	3035.5652	3036.0257
3036.6000	3036.7107	3036.7203

3036.7692	3038.3427	3038.3457	879.5013	879.8579	880.0652
3038.3683	3038.4499	3038.9200	885.7187	901.4224	907.8616
3038.9544	3038.9552	3039.6746	924.8452	938.0099	941.4354
3057.7451	3063.6894	3096.0169	943.8879	945.1617	952.1305
3133.2156	3139.1769	3179.6258	955.5012	956.3722	968.1988
3181.4075	3188.2272	3188.7079	968.3582	971.1461	984.1116
3196.3634	3200.1644	3203.4030	985.3714	989.9317	992.0682
3208.8211	3211.6046	3240.0225	993.0000	998.7808	999.3780
			1003.0298	1004.5200	1006.7722
			1008.4670	1009.3028	1013.1145
			1017.3356	1018.3913	1021.4141
			1024.3346	1025.9738	1029.7123
			1041.4323	1042.7238	1045.3124
			1056.4971	1056.7747	1057.5172
			1058.0131	1058.9232	1060.5155
			1060.8822	1066.0183	1070.8218
			1077.4608	1080.9449	1084.5463
			1089.6935	1091.5090	1098.2287
			1102.1527	1103.4233	1104.8283
			1105.3671	1109.3832	1110.2102
			1111.9685	1115.8315	1116.6630
			1121.9263	1125.9255	1127.8440
			1141.5935	1141.9409	1142.2353
			1143.0220	1145.8950	1147.0917
			1147.8968	1149.4690	1150.7646
			1151.9734	1157.9153	1169.3763
			1174.1739	1175.5156	1178.1144
			1180.0244	1181.3871	1181.7530
			1184.3955	1185.1759	1189.5442
			1190.1531	1191.8060	1192.0858
			1193.1987	1194.4670	1196.0316
			1196.8832	1199.2692	1202.3101
			1207.6159	1211.7235	1212.7548
			1213.7253	1223.9731	1226.7867
			1228.5532	1231.2212	1240.4401
			1246.4582	1288.2418	1290.0609
			1302.4147	1303.9501	1321.4424
			1326.6358	1329.2163	1347.0997
			1357.8225	1359.7881	1363.2909
			1368.1641	1373.2667	1374.1694
			1377.6385	1378.5123	1382.7274
			1387.4080	1399.4348	1401.7196
			1401.8845	1403.5829	1405.2810
			1406.2265	1412.6637	1414.4141
			1417.9753	1424.8356	1431.2049
			1431.8658	1453.8936	1455.6378
			1464.0065	1467.6301	1476.0548
			1483.9614	1485.5524	1486.0799
			1488.1889	1489.0147	1492.0755
			1495.8589	1504.8582	1509.6155
			1510.2450	1514.4257	1519.0517
			1524.3891	1526.0921	1531.0827
			1535.5184	1536.0222	1538.6754
			1539.0243	1541.8382	1548.4509
			1549.7294	1550.5033	1553.5295
			1556.1102	1559.3616	1563.2056
			1565.9952	1570.8547	1576.6826
			1583.5372	1599.8779	1602.8385
			1605.7789	1610.4371	1617.1600
			1624.9013	1627.3945	1627.4566
			1629.9530	1632.0033	1633.8787
			1639.9326	1646.4145	1647.1766
			1651.6964	1656.4402	1658.4889
			1659.9171	1664.7961	1669.8548
			1688.1510	1691.4337	1701.2589
			1707.8041	1712.0327	1716.1830
			1721.8999	1725.4413	1729.8282
			1733.6873	1734.0276	1740.8895
			1745.7998	1755.8105	1758.6054
			1760.3084	1763.7637	1767.6409
			1772.0510	1772.9703	1801.6769

bis-benzophenone singlet		

11.1385	17.7130	17.9992
19.6908	24.3156	30.2405
32.3261	38.4558	46.8270
48.6874	52.2107	55.1936
56.6031	58.1116	59.3734
63.2020	65.3061	66.8133
71.8687	73.8562	75.6005
79.0001	83.7879	89.7290
90.5916	97.6811	99.5214
104.0299	112.9642	116.1514
119.5652	121.7465	128.3181
130.0136	133.0122	139.8331
145.9767	147.5866	161.1599
170.6051	173.9165	181.2190
187.6273	207.2979	209.0824
216.2269	217.4725	219.4027
224.6739	237.5147	240.3837
243.2488	251.5929	258.8193
263.3123	266.1503	278.5719
281.1796	300.0865	306.6730
310.7249	315.6605	335.8472
340.5900	342.9521	347.9306
356.0456	363.4521	366.4665
366.8607	376.4729	385.7709
386.9462	392.0530	397.5495
403.3052	407.7248	411.3573
413.9012	421.0203	425.5904
426.1105	427.9956	428.7746
430.4068	432.1002	434.3513
436.2697	442.0839	443.9551
447.7906	449.7323	453.0879
454.8420	461.7583	463.2064
465.6224	470.7847	478.2805
479.6653	482.4521	489.8411
494.8534	499.8730	510.9391
514.2576	519.4916	521.7797
529.8992	538.0730	548.8471
549.3957	551.6618	569.3105
581.2853	595.7985	599.0881
601.4920	607.1953	613.0945
615.9019	623.1347	628.2867
630.1469	631.1058	632.4570
633.8929	636.2893	637.3345
638.1268	643.9695	645.5395
646.2730	650.6957	660.4402
664.2400	677.3091	681.2841
684.8332	689.4123	695.2414
704.6994	710.7026	715.1130
716.7832	721.7207	723.8298
729.6372	740.1017	747.6192
754.9742	766.4706	769.3187
771.3228	771.3526	776.9570
777.9074	786.3709	787.9780
790.0959	792.5161	797.3376
798.2380	801.6768	804.3907
813.8165	815.2147	830.9736
831.3174	835.7616	838.6815
846.1151	848.5198	861.4470
867.7523	871.5530	877.1164

1803.0628	1824.9845	1825.0819	463.5577	471.2487	473.0765
1829.6733	1829.8496	1856.4673	476.9916	481.7468	488.8099
1856.9854	1858.8703	1861.0771	492.5355	498.0297	508.6624
1901.8495	1901.9911	1906.7589	512.9454	521.6078	526.5896
1906.9087	1922.4351	1922.9305	527.6130	541.9152	548.8038
1953.5602	1955.3166	1973.4192	554.4335	557.4074	571.2830
1973.5188	2050.5786	2051.2921	575.3398	587.7355	595.1159
2062.4718	2069.2762	2841.4805	598.4797	602.0803	611.1437
2844.9595	2846.8472	2851.5553	616.3093	618.7990	622.5508
2853.4587	2854.9318	2857.2270	625.0112	630.8778	632.2714
2857.7779	2862.2977	2864.3370	633.4995	634.9621	636.2539
2868.7187	2876.2876	2936.6018	637.1481	639.0524	640.4442
2938.4925	2941.4356	2942.6374	641.5575	644.2287	647.6596
2944.7683	2946.2216	2947.1262	662.6790	675.5004	676.9542
2949.7711	2952.2832	2952.5687	682.7327	692.5899	696.1449
2954.4172	2955.7094	2958.0487	706.2128	709.0464	717.7857
2959.6431	2962.5948	2964.2801	722.9132	724.0384	725.7345
2974.2315	2976.5396	2981.1499	731.7532	738.1667	746.6715
2982.4611	2985.9424	2992.5086	751.0595	763.6488	767.3232
2998.9456	3007.0861	3033.8411	771.6355	771.6931	777.2372
3033.8847	3034.0117	3034.5940	777.6390	778.2400	782.3490
3034.8750	3034.9006	3035.0545	789.4122	790.2977	794.2675
3035.2831	3035.5762	3035.7483	800.3841	803.2214	806.0701
3036.9550	3037.0789	3037.5719	814.1754	815.1667	830.9355
3037.6570	3038.4473	3038.4742	831.4973	835.5287	838.4088
3038.7024	3038.9241	3039.2678	846.9501	850.2161	867.2815
3039.4943	3041.7119	3042.5579	872.8584	874.7458	879.7566
3059.4383	3079.7353	3124.9532	880.8686	881.5401	883.7593
3148.6304	3184.1939	3184.5313	886.0831	901.3149	908.0880
3185.9522	3186.1661	3191.4507	930.0108	935.0732	937.4813
3193.8994	3196.0386	3197.2878	943.6081	944.4926	952.6831
3199.9382	3207.3765	3207.7986	954.2594	959.0235	967.1173
3209.1318	3210.1041	3215.2091	970.4556	979.0383	982.4553
3215.5673	3221.3542	3222.2505	988.2450	992.5075	993.9972
3252.5339	3263.2867	3274.9196	996.4505	998.8490	1002.9598
----	----	----	1006.4758	1007.5613	1009.0029
bis-benzophenone triplet	----	----	1011.6706	1014.4436	1015.9476
----	----	----	1017.9521	1019.7369	1020.2465
13.4734	14.8686	17.0888	1025.7320	1030.5531	1034.6155
20.8920	26.0775	28.9764	1041.3246	1042.3773	1047.4098
31.4537	39.2111	44.7677	1055.2802	1055.5891	1056.8386
46.1382	50.4181	53.0647	1057.3940	1058.7321	1059.2331
54.2954	57.8326	59.6681	1063.2265	1064.9786	1069.0750
61.5755	65.6446	71.8197	1075.6696	1081.3329	1084.1521
72.2631	74.7910	80.1930	1087.8840	1093.7382	1094.0265
81.8660	85.9383	88.0295	1103.1285	1105.3701	1106.6107
90.4586	97.1532	98.8434	1107.6130	1108.3988	1109.5872
107.8418	109.4630	114.2396	1113.3777	1113.7947	1117.7728
121.4739	124.5949	127.2795	1118.8724	1123.7931	1126.0617
132.8361	136.6599	141.0075	1142.1396	1142.4135	1143.3050
145.2618	148.2316	160.7707	1143.3910	1146.2336	1147.4375
171.2420	172.1611	175.1659	1148.1480	1149.5504	1150.6583
185.8665	192.7958	204.1798	1152.5948	1157.3048	1165.5654
211.4401	214.4614	216.0252	1174.8966	1177.3277	1179.5606
218.9758	223.7211	234.0032	1180.2319	1181.5374	1182.2719
238.4797	241.3083	247.4188	1185.1752	1185.8488	1186.9872
257.0762	267.8364	271.5797	1189.5392	1192.4388	1193.0515
279.0274	296.8628	297.6205	1193.2179	1193.7406	1194.7212
300.2064	311.0172	317.1849	1195.4444	1198.5635	1205.3433
334.6582	336.8845	339.6268	1206.8243	1210.5098	1212.0758
346.8547	351.1670	362.2656	1213.0231	1221.8534	1222.7988
363.0045	366.0094	379.4772	1225.3658	1228.2756	1243.3643
381.1806	383.1600	388.3235	1245.7762	1288.1663	1290.1219
389.4418	404.5633	407.8099	1302.3958	1303.8421	1304.8122
416.6059	423.3216	426.2870	1312.5226	1320.0501	1337.5190
426.3586	427.4633	431.8212	1348.3162	1354.1508	1364.1005
433.5461	435.0566	435.7207	1367.4503	1368.7828	1373.1456
438.9917	440.5636	444.2198	1374.6544	1375.4239	1376.2163
447.7716	450.2414	452.5824	1382.3524	1385.2995	1399.6962
452.6549	454.4178	461.8445	1401.8194	1401.9510	1403.8635
			1404.6517	1405.2227	1410.6278

1413.7134	1419.1445	1425.1141	64.2984	66.4839	74.1549
1432.5678	1434.0412	1457.2151	75.5113	76.9770	81.2416
1466.3069	1467.5445	1472.3560	82.1384	88.5694	90.1834
1479.0755	1483.1310	1483.8571	96.9476	98.3633	102.3915
1486.1271	1488.0246	1490.2969	111.1305	113.3354	117.4947
1496.2111	1498.7153	1503.7608	122.4940	123.3679	129.6788
1508.5771	1512.8117	1518.7599	132.8002	139.6058	140.2710
1524.0602	1524.2833	1531.5497	148.0297	153.6654	158.4323
1534.6824	1535.9708	1538.3261	161.3830	170.3181	172.8064
1539.5092	1540.1638	1547.2662	182.3042	194.5749	195.0261
1551.7074	1553.5761	1555.2391	210.9904	212.2482	216.0022
1558.4870	1560.4643	1562.8226	218.8017	227.7634	237.2011
1563.7487	1571.9409	1574.8673	240.5493	245.0664	252.2599
1584.9952	1598.4506	1607.0156	257.3226	264.1836	267.8021
1609.8309	1614.7093	1615.4380	277.1536	284.7820	298.8561
1616.2270	1624.3615	1625.9759	301.0429	308.0062	326.5000
1626.9654	1630.9008	1631.7739	338.2565	346.0883	348.7702
1641.0378	1642.6279	1647.4084	354.1626	357.4673	362.4329
1647.6534	1648.4251	1655.5540	367.0580	377.3299	379.4320
1656.8008	1666.5993	1671.0318	380.9419	389.1672	391.5989
1687.5477	1692.0980	1702.0102	399.0406	405.1142	407.9639
1707.6370	1712.3883	1715.7955	417.1767	425.7923	426.4874
1722.3497	1724.9639	1731.3989	427.9707	428.8456	433.7014
1733.3269	1734.7899	1741.2515	435.1199	436.3558	437.8104
1744.6561	1756.9698	1759.8915	440.0985	444.2970	446.1239
1762.1798	1763.3715	1773.1834	449.0300	451.8802	454.2406
1773.2742	1773.5072	1802.4998	454.8136	455.3240	462.0818
1804.7520	1825.0737	1825.5315	462.6765	470.4050	472.2842
1829.8343	1830.2330	1856.9617	475.6563	480.9880	488.1519
1857.2377	1859.5210	1861.7063	496.0266	497.3832	509.2219
1902.1177	1903.0012	1907.0023	512.7205	520.8084	521.3970
1907.7122	1922.2221	1925.8856	527.2654	539.1120	548.2196
1953.1758	1956.0369	1972.6661	551.9678	553.8699	567.4645
1973.2775	2050.8969	2051.6955	570.6415	589.4053	589.6278
2062.9018	2064.1767	2840.4955	596.4177	600.0199	602.8297
2843.9355	2846.0645	2850.7224	612.6795	619.0172	621.3359
2852.9064	2854.2900	2856.6566	622.5559	631.5165	632.7564
2856.8794	2858.3269	2861.2410	634.2663	634.7635	635.1582
2867.1345	2871.4733	2936.2919	636.3375	639.4700	641.2282
2938.2779	2941.6214	2942.5654	643.4821	644.5623	647.7107
2945.0526	2945.5576	2946.7944	664.0228	677.4083	681.2958
2949.1413	2949.7355	2951.3633	695.8504	696.8449	700.5042
2953.1531	2954.0305	2955.3607	709.4280	710.8748	719.0036
2957.5026	2959.8090	2963.2084	723.7905	727.3094	728.0766
2972.4937	2974.2308	2977.6702	732.3915	739.5369	741.1698
2977.7512	2979.6840	2987.3799	745.0593	762.1254	766.1635
2993.9701	2996.6033	3033.7165	770.9359	772.0607	774.1878
3033.8530	3033.8880	3034.7842	776.3162	776.5738	781.9922
3034.8145	3034.8692	3035.1049	785.5353	787.7083	790.3449
3035.2957	3035.6299	3035.7786	793.2547	797.4909	814.2906
3036.8089	3037.0633	3037.6434	815.2327	830.7384	831.0515
3037.6486	3038.3923	3038.4902	832.0392	835.5615	837.6419
3038.7005	3039.0742	3039.0998	846.2273	847.8711	869.3700
3039.4312	3042.1570	3043.4339	878.7788	879.8289	881.3063
3062.0933	3073.1171	3134.5772	882.0588	885.2045	888.4481
3154.9836	3180.5492	3181.5330	892.2487	901.2231	907.1677
3186.7400	3188.0142	3188.8629	930.4787	940.0401	943.6844
3189.8684	3197.0687	3197.1845	943.9768	944.8910	948.0057
3199.1496	3203.0416	3206.6065	965.0082	968.7244	970.5712
3209.9638	3211.3726	3211.8591	974.8802	976.5589	986.7714
3222.4503	3225.6311	3237.3115	992.5291	996.5773	998.8175
3252.3564	3259.5427	3279.7268	999.5649	1002.7861	1003.6787
			1007.9467	1009.4403	1010.7959
			1012.5279	1016.6050	1018.1926
			1020.0848	1024.6230	1026.3985
			1028.3848	1033.8808	1039.2928
			1041.0800	1043.9932	1046.8861
			1055.0395	1055.7406	1056.4353
			1057.0549	1058.1304	1060.8058
			1063.1763	1064.2083	1068.4052
			1077.1390	1081.6639	1082.2761

bis-benzophenone quintet

12.8333	15.1981	19.2404
25.7926	27.5711	31.2035
38.6355	45.1068	48.2016
50.1574	52.8740	53.6694
55.8618	58.8790	61.7447

1086.4849	1092.1092	1092.9799
1102.8343	1104.7581	1106.4600
1107.6122	1109.1824	1113.5914
1114.7288	1116.5741	1117.6144
1119.5374	1121.7022	1129.4181
1142.1014	1142.2906	1143.5126
1144.3049	1145.3603	1146.6682
1149.3135	1150.0782	1151.9183
1152.3051	1155.7381	1165.7613
1167.4063	1173.9949	1177.3682
1180.0898	1181.1919	1182.3688
1185.1208	1185.5837	1186.6359
1187.2078	1190.7593	1192.6704
1193.4085	1195.3288	1195.5437
1196.0262	1198.5824	1200.7322
1208.1253	1209.0238	1212.7866
1214.8205	1221.4068	1224.9605
1226.1407	1228.5533	1243.8442
1252.5256	1288.4230	1290.6946
1294.6248	1304.2681	1306.5874
1309.1205	1313.7024	1338.9421
1353.2176	1359.4435	1360.3788
1365.8837	1370.8115	1373.1658
1374.8844	1376.6670	1377.0089
1382.5719	1383.6326	1400.5304
1401.5440	1402.0713	1402.3290
1403.8901	1404.6088	1412.0337
1413.9393	1421.7333	1423.2804
1430.6420	1433.3571	1458.5055
1463.9212	1467.3188	1480.1994
1481.2271	1482.8702	1485.3241
1485.9463	1489.3654	1493.7868
1495.9478	1496.1983	1506.3001
1509.9323	1510.5508	1519.1456
1523.8446	1524.5167	1533.1639
1534.6720	1535.0152	1536.4509
1539.5535	1542.4730	1546.6594
1551.5858	1554.4529	1555.3162
1560.4114	1564.5110	1565.2604
1571.7041	1574.5685	1581.5044
1584.5401	1601.7417	1610.0639
1610.2535	1612.0813	1615.7303
1617.1286	1623.8057	1624.6601
1630.4877	1634.2353	1637.2724
1640.4215	1641.3886	1648.5214
1649.5737	1651.5839	1656.8657
1666.4024	1667.2464	1670.2666
1688.0109	1692.5716	1702.5527
1709.1752	1713.5880	1715.9255
1723.0387	1724.7446	1732.0127
1735.0910	1736.7207	1739.9554
1746.8712	1757.4334	1762.7694
1762.9159	1768.4065	1773.0127
1773.5239	1775.0629	1806.1980
1806.5171	1825.2681	1825.6929
1829.9261	1830.2677	1856.9913
1857.5614	1861.0198	1861.6880
1902.4616	1903.3529	1907.6883
1907.9719	1926.9265	1927.3058
1954.8703	1957.0267	1973.4945
1973.6255	2052.3075	2053.5173
2063.8337	2070.4058	2840.4384
2844.9091	2848.3743	2850.6082
2852.8423	2854.5584	2856.5236
2857.3743	2859.7726	2861.1971
2866.2307	2871.2024	2936.2572
2938.3220	2941.6639	2942.4919
2944.3506	2945.7787	2947.4027
2949.4232	2950.6020	2951.5667
2954.6170	2954.8683	2957.0448
2959.2117	2961.3220	2962.4635

2971.2221	2973.3455	2975.2331
2977.3638	2978.9249	2986.8760
2993.0760	2994.9373	3033.5803
3033.6834	3033.8013	3034.8042
3034.8212	3034.9667	3035.1500
3035.3147	3035.8361	3035.8423
3036.7618	3037.0249	3037.6389
3037.7085	3038.3722	3038.4859
3038.7845	3039.0319	3039.2829
3039.6404	3043.2491	3049.2206
3063.6227	3069.2509	3139.2627
3163.7848	3176.7182	3177.6204
3185.7819	3187.3563	3192.5514
3193.9857	3198.3365	3204.2876
3205.1848	3206.3339	3206.6584
3215.0405	3216.4226	3220.0770
3227.2409	3228.9508	3251.0507
3260.1057	3260.7436	3268.9286

benzophenone transition state triplet

-1016.3880	11.8243	14.9149
17.4627	20.1587	29.9766
34.9824	38.0124	45.3374
52.2736	52.7665	53.0411
55.4645	57.6958	60.2190
64.3455	67.7468	69.4884
74.7052	77.1070	78.0698
82.5496	83.5266	88.5331
92.4722	93.0618	97.4866
104.5351	106.7574	112.7994
115.6030	118.3912	119.8141
129.2195	135.4828	144.6379
147.3478	158.3540	161.9631
169.5557	175.3153	177.5525
192.2213	204.2009	212.5263
214.3723	217.4335	220.9056
226.9872	233.0365	240.1640
242.0810	258.9094	262.4604
264.5599	272.3364	281.9204
292.6149	295.1340	305.1407
316.3202	325.5071	334.9553
338.4545	350.4112	354.1971
365.1303	368.7501	371.5884
374.6132	384.0188	384.8572
403.9594	408.8826	413.5627
417.2576	422.8756	424.1190
424.6917	425.8784	427.3991
427.7751	429.3240	432.9666
434.6305	436.9630	438.4916
442.3910	446.2408	450.5663
455.1165	456.5473	458.8217
460.5479	461.9981	468.3624
476.3234	480.0026	487.9902
495.8000	497.1393	499.2914
506.1472	508.1390	510.9050
516.2836	520.9320	523.8735
524.8152	545.6490	549.9711
552.4442	556.3684	570.5524
578.6270	584.0726	591.1031
597.2731	602.4270	607.9358
610.4747	616.8644	623.5135
633.5920	635.0372	635.6157
636.3696	637.0646	638.0556
640.3913	640.8814	644.7686
646.7064	651.1769	669.4128
679.6960	682.4246	685.5701
690.2572	690.2739	701.9212
708.7967	709.7647	715.8628
719.3940	723.4933	727.9443

731.2194	732.7175	743.2247	1640.0146	1640.6654	1643.6657
764.0096	765.4250	769.0114	1652.9452	1653.8147	1657.8036
770.0290	770.7915	771.5897	1659.0892	1664.7877	1669.8294
773.0837	775.7132	782.0731	1684.3882	1687.4075	1700.6227
783.2400	784.7154	800.1906	1701.4112	1709.0498	1712.8483
803.2907	812.4166	812.5291	1716.1594	1717.6829	1722.5463
814.4792	824.1960	829.1764	1724.3237	1729.0080	1732.2610
830.1166	836.8587	838.7318	1741.6675	1754.1714	1761.3004
846.2242	852.6789	863.8794	1762.4211	1767.4417	1768.0298
868.2419	870.8851	875.5358	1769.3914	1785.1931	1787.6338
878.8639	879.0375	880.3139	1801.4355	1823.2307	1823.8300
882.1491	899.1963	900.1749	1828.0942	1828.2138	1851.8271
912.2181	928.6181	939.5743	1855.6821	1856.7927	1856.9377
942.4830	943.8113	944.4410	1894.0969	1898.6539	1901.4816
949.0638	958.1287	968.6978	1903.0374	1907.3747	1912.8424
971.7434	980.6084	982.2134	1948.4780	1951.8707	1969.3337
983.4496	988.3023	993.3660	1971.1362	2041.3155	2045.1494
996.0254	999.5474	1001.4018	2049.4949	2054.7727	2839.8789
1002.1024	1005.1344	1006.0780	2841.0997	2846.0925	2851.3980
1006.9105	1007.9429	1014.9556	2851.8581	2853.8757	2857.3372
1018.3330	1019.0549	1019.8118	2857.9029	2858.3573	2859.0429
1021.9091	1022.2870	1026.7341	2861.9924	2862.6108	2936.9950
1029.8707	1035.4799	1039.5826	2937.8240	2940.0025	2941.4173
1044.0460	1053.9544	1054.4912	2943.4328	2944.3496	2944.6868
1055.3342	1058.0523	1059.0683	2947.9253	2948.0909	2949.4857
1062.6658	1067.1949	1067.9658	2950.6169	2952.2999	2953.4107
1074.4378	1079.6522	1080.4940	2956.2077	2960.5922	2966.1323
1083.4894	1085.3143	1089.8469	2967.8145	2972.4462	2973.3142
1094.2103	1100.9060	1102.7407	2978.8814	2983.1803	2989.0122
1103.2327	1103.8050	1105.5805	2989.2809	2994.7225	3033.8622
1110.0257	1116.3739	1117.8330	3033.9148	3033.9618	3034.0818
1118.6810	1119.1537	1122.3878	3034.8971	3034.9529	3035.0469
1133.8500	1139.2023	1141.5169	3035.1102	3035.7423	3036.4220
1141.9287	1142.2761	1143.5782	3037.0222	3037.1189	3037.3445
1145.1936	1145.7299	1146.3690	3037.3972	3038.4525	3038.4652
1148.8464	1149.3274	1156.8089	3038.5431	3038.5553	3039.3639
1165.2809	1166.3646	1169.6552	3039.5916	3039.8074	3040.9894
1175.1257	1175.9365	1177.3008	3042.2256	3056.0800	3082.1596
1178.9883	1182.4172	1184.9948	3165.3190	3182.1824	3182.2981
1191.1526	1192.0957	1192.7819	3184.2651	3185.0409	3191.3122
1193.5557	1196.8996	1197.2451	3191.8129	3199.0144	3199.0451
1197.3281	1198.4908	1201.4741	3206.4490	3207.0056	3211.2253
1209.4694	1210.8250	1213.8516	3212.0281	3224.8061	3227.8781
1217.0988	1224.4174	1226.4457	3238.8392	3263.5845	3270.0620
1227.4532	1229.1608	1230.0643	3271.9223	3272.2779	3289.2306
1236.4447	1238.5442	1240.4544			
1241.6212	1279.1113	1287.7944			
1288.3195	1297.8044	1299.5797	----		
1333.5282	1335.7427	1345.9578	benzophenone diolate triplet		
1348.7348	1365.2794	1366.2398	----		
1370.3244	1372.2592	1372.8805	11.3455	15.1544	18.5826
1373.3150	1379.2613	1379.9215	19.9865	34.5056	35.9478
1401.0944	1401.3875	1401.9036	38.3522	44.6942	50.1596
1402.0110	1402.4443	1408.8700	53.4078	53.8643	55.0106
1413.7909	1420.3560	1421.0861	60.1267	62.2498	63.4152
1423.3287	1428.9010	1439.4544	67.0178	68.5548	75.8548
1463.6224	1466.1501	1470.3970	76.9071	79.0075	80.4636
1482.3843	1487.4712	1488.4295	84.8247	85.0660	87.4271
1492.4406	1493.5608	1494.7432	90.0691	95.4132	101.4268
1497.0758	1500.8505	1502.7901	109.5729	113.6004	115.8776
1508.6489	1512.3004	1515.8407	116.5046	120.8826	130.6058
1521.5865	1525.5225	1528.6514	136.0565	143.1562	160.3416
1533.7502	1535.7842	1537.7282	164.2639	164.9117	177.0950
1539.2972	1541.6054	1546.1481	182.2579	191.9653	197.7873
1547.5698	1549.7238	1552.4015	208.5313	214.2190	220.4558
1556.4906	1557.7855	1561.6217	222.2160	223.9945	236.9502
1569.5737	1572.5880	1581.4453	238.4658	241.6384	247.6433
1590.0785	1595.5106	1600.0674	263.4264	264.4953	272.5415
1603.2694	1614.0115	1618.8137	279.7057	284.9418	295.4955
1632.1432	1632.2752	1632.4829	301.0921	305.0330	310.5183
1635.2357	1636.7727	1637.3413	324.8511	338.7958	346.3761
			352.4253	360.5928	364.3325

369.3451	374.1709	380.7315	1221.1294	1223.1854	1228.5092
384.8688	389.6685	396.4202	1231.1137	1231.5346	1235.8720
408.4113	416.8650	418.2137	1238.6153	1266.2816	1287.9854
420.8280	421.6645	424.5875	1288.1382	1296.4189	1299.6622
425.4131	426.6328	427.7967	1334.9391	1336.6331	1342.5438
428.7392	429.9834	430.6731	1345.0235	1362.9435	1364.6524
437.5201	442.0092	443.3195	1371.5046	1371.8225	1372.3669
446.7156	451.1839	454.9556	1372.8067	1378.7179	1379.9941
455.9830	460.4160	465.4427	1400.9000	1401.3200	1401.9617
474.1176	478.5402	479.5414	1402.1248	1403.5118	1407.8613
482.8771	484.2307	490.3832	1414.7068	1418.5230	1421.9974
497.8818	502.9008	505.6227	1423.3590	1429.6389	1437.6105
509.5900	513.4065	518.1455	1463.4184	1467.1573	1473.2642
521.0458	523.9190	539.3751	1484.9395	1488.3647	1488.8467
548.0280	550.4952	554.4377	1492.2213	1493.6490	1493.7347
559.1945	570.3030	573.9213	1498.8164	1499.4617	1503.3140
580.1779	583.8937	594.8200	1508.1758	1508.6998	1520.6092
604.4814	608.8310	611.6501	1524.6037	1529.3629	1531.0895
616.0507	624.2839	634.3687	1534.8849	1538.2894	1538.5205
635.4189	635.6804	636.8790	1540.1166	1541.4968	1543.6822
637.8096	639.1093	643.2398	1545.8047	1549.0174	1550.5995
646.0248	651.6937	658.3811	1554.9921	1557.2677	1563.7490
659.7813	666.3210	674.6334	1567.7462	1573.4829	1582.1297
682.3034	683.0402	690.4499	1589.8856	1594.2071	1598.9316
691.1153	710.4802	711.8779	1600.6986	1614.3129	1615.0183
715.0677	721.5203	725.9551	1628.6025	1634.1691	1636.9268
727.0172	732.0494	740.5993	1637.7858	1637.8364	1638.9055
746.2974	761.1769	766.7515	1639.6143	1639.9662	1642.2145
770.6584	770.9564	771.9893	1657.1957	1657.6758	1660.0626
772.6814	778.0427	778.7896	1660.9799	1664.1639	1668.3049
781.1055	783.2572	783.9862	1682.0081	1687.4412	1699.0269
797.1682	807.2007	812.6831	1703.6394	1706.4716	1712.0523
813.7536	817.1000	822.7623	1715.9806	1716.3878	1719.4336
830.9295	831.8214	837.6455	1724.1541	1727.1896	1730.5552
839.7457	852.5201	854.5847	1741.6001	1755.6394	1759.9737
863.2154	864.9416	868.4889	1760.4709	1765.7500	1768.0739
869.4841	872.8184	878.8284	1773.8986	1782.2873	1784.3715
879.2030	881.5763	881.7567	1799.1098	1823.0002	1823.7103
893.1755	899.8832	903.2068	1828.0177	1828.2048	1851.0936
924.7296	933.5649	937.0158	1855.3317	1856.9501	1857.0384
943.6319	943.9109	948.2051	1891.8696	1898.2086	1900.7343
969.3735	970.0056	973.4392	1902.9664	1905.4885	1911.8123
976.4647	978.7149	979.8505	1947.1020	1951.0209	1968.4804
981.9803	984.5711	994.2862	1971.2566	2038.5767	2044.4130
996.1055	999.3905	1000.1349	2047.6910	2055.3096	2839.9804
1001.5734	1003.6611	1007.8517	2841.3952	2844.7147	2852.9786
1008.1460	1009.0795	1009.6364	2854.0373	2857.0203	2857.7480
1011.8706	1017.8902	1020.4276	2857.8892	2859.2550	2860.3360
1021.1402	1022.3439	1022.8807	2861.1687	2861.2985	2937.5733
1023.9674	1027.6521	1032.8531	2938.4046	2940.4583	2941.9044
1044.3738	1047.5881	1050.9167	2943.2768	2943.9556	2944.2756
1055.1305	1058.3958	1060.3942	2948.4066	2949.3742	2949.8962
1062.2525	1064.0548	1064.8365	2951.0787	2952.0539	2955.1440
1069.6232	1073.4775	1078.6065	2956.4304	2958.1090	2967.6461
1080.3653	1081.5174	1086.2746	2971.4787	2975.0087	2975.1089
1088.1387	1089.2587	1101.9044	2978.2754	2981.7092	2988.0370
1102.7566	1103.3987	1104.5383	2992.1294	3003.9488	3033.7296
1107.0753	1113.5281	1114.7809	3033.9798	3034.1385	3034.2588
1117.2138	1118.1083	1125.4253	3034.8111	3035.0202	3035.1439
1129.2738	1131.6852	1141.6165	3035.1695	3035.7406	3036.5731
1141.9284	1142.3117	1143.4484	3036.8589	3037.3802	3037.4824
1145.3333	1146.2078	1146.7975	3037.5342	3038.4028	3038.5676
1149.3422	1149.7134	1156.5048	3038.5789	3038.6874	3039.0875
1158.4821	1166.1290	1167.0267	3039.8388	3041.7381	3042.0450
1169.9060	1173.8676	1175.1185	3052.7038	3068.1302	3084.7596
1176.5377	1178.6325	1179.3504	3154.0208	3180.1990	3180.5493
1180.8327	1188.1604	1188.4601	3181.3157	3181.5754	3189.2310
1191.8313	1192.6412	1194.7659	3189.9711	3195.5349	3197.0764
1196.3634	1196.6487	1197.7146	3203.7263	3205.3360	3208.6523
1198.2600	1198.8184	1205.2979	3212.0612	3213.0275	3225.1049
1210.4271	1212.2584	1217.5943	3238.6046	3264.8554	3266.4349

3288.3009 3297.2573 3299.8035

mono-benzaldehyde triplet

10.8198	13.7966	19.0628
24.4921	31.1852	41.0498
48.0013	49.7415	53.2034
54.4942	56.4169	58.8140
64.4496	71.7110	76.3190
80.1972	85.7686	91.0457
93.6962	100.0654	101.5631
109.3451	115.0813	123.5460
129.9957	134.5677	137.7825
152.7348	156.0853	166.0562
174.7987	190.0722	193.6989
203.5574	211.1794	213.7253
238.0578	239.7988	241.1314
258.6625	260.8555	283.5010
294.8835	299.1623	307.1918
317.5088	329.2483	332.2292
335.3571	348.5559	349.8460
363.1036	374.3351	384.2090
386.0608	388.8440	390.9629
396.5181	405.6506	411.6745
413.3916	416.2954	424.7578
426.4932	428.4944	428.6272
432.2567	439.8851	441.6679
442.7924	446.3875	452.8972
457.0689	457.5467	465.1712
472.2473	475.1765	478.1388
481.0658	493.3575	496.9837
511.0922	514.9780	518.9015
523.7520	538.1082	549.7437
551.4097	551.6845	562.5624
570.9229	580.0983	588.3393
594.5138	598.0075	604.6264
612.6620	615.3487	623.0665
626.8091	630.4704	631.7693
650.5429	663.7108	665.6298
673.2479	674.5538	689.1626
692.6764	694.1178	706.9713
710.0155	725.0766	733.2354
748.9262	760.8364	762.0891
767.5904	768.2758	778.9236
780.4707	781.9229	800.1123
804.2436	812.2841	812.9493
816.4864	822.4566	829.3242
830.5452	836.7148	837.8176
838.2684	846.2343	849.2833
855.4241	878.5550	879.4580
879.6443	879.8436	901.6441
905.2723	909.3784	943.5404
944.0531	960.9349	961.9943
965.4814	992.3775	993.2885
994.4007	998.3395	999.0177
1004.2550	1007.5441	1010.3368
1017.4024	1025.0660	1029.9186
1030.2816	1036.4161	1041.4794
1043.3195	1049.2300	1055.5357
1056.2175	1061.8019	1063.3280
1074.5542	1078.1312	1081.1215
1081.4731	1090.8091	1097.1102
1101.9800	1102.5724	1103.0934
1104.6076	1104.7995	1106.2083
1118.9377	1127.7185	1141.6331
1141.9641	1142.3339	1142.4648
1143.0635	1145.4642	1145.7294
1147.7259	1148.5291	1150.0001
1161.2151	1163.9711	1167.0037
1174.6825	1175.1768	1177.2370

1178.4815	1180.4542	1181.2406
1181.9648	1185.1895	1189.0215
1191.0084	1196.7677	1197.6428
1201.4488	1204.6282	1216.2639
1221.2125	1225.4328	1236.6454
1248.6537	1254.7691	1288.7706
1289.8204	1299.7765	1300.6644
1344.4370	1358.0083	1372.6317
1373.1907	1375.1962	1379.6249
1381.6570	1401.3336	1401.6991
1402.0293	1402.2366	1403.6632
1404.5783	1405.2344	1413.8613
1416.2000	1419.7410	1431.5073
1432.8249	1453.8339	1456.2347
1459.4218	1472.6189	1474.2378
1480.3431	1481.5440	1486.6012
1489.7101	1494.9324	1503.9350
1504.8159	1508.6792	1515.1953
1517.5435	1524.3207	1526.3136
1533.2731	1536.6257	1539.7987
1543.8562	1547.6838	1554.1506
1555.1309	1556.6816	1563.2377
1570.8276	1575.2398	1577.7920
1583.7271	1592.6060	1598.0737
1598.9086	1599.5911	1602.6978
1619.1543	1625.4732	1627.2087
1639.6016	1641.3165	1642.1088
1663.4498	1665.4782	1685.9408
1688.3693	1698.2783	1702.1175
1703.2788	1708.7828	1714.4840
1716.2205	1724.1561	1728.6666
1728.9912	1730.5467	1744.9490
1746.2736	1751.6995	1753.6870
1755.7069	1763.3070	1768.1086
1769.4977	1791.4405	1802.3209
1823.7914	1824.1007	1828.0958
1828.4173	1854.9792	1856.7092
1857.3507	1857.4976	1898.7528
1899.6952	1903.4953	1903.6331
1915.0504	1915.5836	1950.8527
1952.4975	1971.4208	1972.5360
2047.0262	2048.5734	2056.4645
2059.8621	2840.9126	2841.4430
2842.5719	2847.5788	2849.4691
2850.8272	2853.0248	2854.0497
2854.7313	2860.8411	2863.8108
2868.8483	2937.8317	2938.6780
2939.8469	2942.3729	2942.4211
2944.6802	2945.3869	2946.2233
2946.6495	2948.0209	2948.8492
2950.7165	2952.1538	2958.1993
2959.4396	2961.7243	2968.3570
2969.2940	2973.0657	2980.1049
2980.6439	2981.5478	2985.3554
2999.6193	3033.5502	3033.5871
3033.5999	3033.6580	3034.7000
3034.7617	3034.7849	3034.8534
3035.5560	3035.6946	3036.4166
3036.5981	3036.6877	3036.7310
3036.9059	3038.3286	3038.3535
3038.3563	3038.3718	3038.9290
3038.9349	3039.0037	3039.0840
3049.9239	3091.6540	3114.5455
3152.5199	3182.6659	3192.3259
3201.5254	3214.4045	3227.3411

mono-benzophenone triplet

10.4126	13.3696	16.7716
19.8759	26.7169	27.3117

35.6374	39.1035	42.7419	1183.9637	1186.2333	1187.1970
47.9758	50.7923	55.3679	1188.3018	1194.7442	1195.6841
55.9274	57.4184	63.7308	1204.9061	1207.9691	1209.4754
70.6153	72.4805	76.0552	1213.4294	1215.3949	1224.7223
81.9900	83.7755	86.6188	1225.2971	1226.6003	1242.4645
92.4223	97.3923	102.6006	1247.8689	1287.9168	1288.1388
109.6958	117.9853	127.3972	1300.0262	1302.6805	1321.7184
130.1110	134.7192	143.4889	1327.6140	1352.6703	1369.9892
151.3719	154.5609	161.6695	1372.1362	1372.9473	1373.3450
166.0804	190.4682	199.3126	1379.8913	1382.0005	1384.2843
202.1569	210.5617	212.7384	1401.7074	1401.9164	1402.1479
221.0466	223.6115	228.3908	1402.7480	1403.8196	1404.6637
251.3004	257.2643	261.0197	1409.8564	1412.6879	1418.4945
295.5937	297.3296	299.5450	1419.4556	1431.1168	1431.7200
306.4770	316.9651	320.9959	1458.4511	1459.6124	1476.9096
327.0241	336.4496	345.4829	1479.9502	1482.2860	1484.2905
356.7170	361.4174	367.6098	1488.9602	1489.2530	1491.8702
370.7239	375.2952	378.1389	1498.2078	1499.2089	1500.1331
384.5913	387.8696	394.9946	1506.6319	1508.0418	1521.0088
408.0495	414.7231	418.4925	1521.7119	1531.6082	1533.4870
420.2996	424.0179	425.5271	1534.6502	1535.1664	1536.9324
426.3457	429.0011	431.6870	1540.0447	1549.0763	1549.4645
432.5084	438.3596	440.0503	1552.2573	1556.1945	1564.9685
446.3431	447.4074	449.7896	1566.3390	1575.5032	1578.2342
454.1043	454.9038	462.7815	1590.0986	1590.8727	1599.0650
465.3389	473.6386	475.9895	1602.5243	1604.4662	1606.3574
489.3217	492.4591	494.9063	1621.4106	1625.8917	1626.2190
498.8032	501.0452	510.9089	1627.0882	1635.3094	1639.2369
514.3707	531.7313	540.6803	1643.6827	1652.2620	1662.2040
549.9383	551.1227	567.8591	1664.6412	1685.4990	1687.3797
570.9573	576.9900	585.6109	1698.8038	1700.7720	1701.1944
596.5828	600.0802	602.3666	1705.3561	1714.8334	1715.8897
604.6187	619.0836	627.5270	1722.3234	1725.8844	1726.5993
628.7812	629.9356	631.3858	1728.4819	1748.0208	1748.2068
632.7509	634.7452	641.7255	1752.0943	1755.4391	1759.1342
642.9541	646.2289	659.4641	1760.2738	1766.3515	1769.8010
684.6677	688.4015	690.2190	1790.9881	1794.5084	1824.0066
691.3266	705.3811	706.5129	1824.3602	1828.5928	1828.7835
709.4222	723.7375	728.9599	1854.8705	1856.9797	1857.1527
733.6986	751.9562	760.1439	1858.5790	1896.7733	1900.6060
762.2113	769.9958	770.6006	1902.6211	1903.8053	1909.5744
776.8036	779.2882	783.0679	1915.6474	1949.8734	1951.2184
793.9465	795.3111	795.6982	1970.8487	1972.9911	2042.6806
812.5968	813.0964	813.6681	2045.5979	2054.4049	2059.3276
820.5074	829.9700	831.0989	2839.7313	2840.2132	2841.5998
837.6109	838.6520	854.3514	2846.5105	2848.3553	2850.0434
859.0655	865.0269	879.4601	2853.4862	2854.6330	2855.5521
879.6728	880.8496	882.2654	2858.7262	2859.4361	2860.6000
886.0493	901.1307	904.6192	2938.6405	2938.7693	2939.8771
931.6125	943.6696	944.3781	2940.3074	2943.6302	2944.0345
946.6534	953.8501	956.5422	2944.3235	2944.9836	2946.6814
961.5650	976.0493	989.6606	2948.1983	2948.3907	2948.9477
990.1258	993.1289	997.1311	2950.9491	2957.2540	2957.6743
999.3068	999.5521	1002.7698	2958.9426	2962.0210	2966.2901
1004.0326	1010.4916	1010.7048	2970.5941	2972.6249	2978.1092
1013.9434	1015.2966	1026.4009	2979.0998	2985.1324	2986.8123
1029.5523	1031.0898	1043.2393	3033.5634	3033.9280	3034.0898
1045.1619	1055.3974	1057.9641	3034.1374	3034.7234	3034.9403
1058.3162	1060.1478	1060.9180	3035.2913	3035.2954	3035.5921
1064.4647	1072.8488	1075.5780	3035.9167	3036.6965	3037.1020
1080.2851	1081.6251	1085.6564	3037.1321	3037.4258	3037.7846
1088.4725	1102.5543	1102.9646	3038.3422	3038.4946	3038.7122
1103.9476	1104.4795	1105.2546	3038.7756	3038.9297	3039.5424
1105.9223	1118.4524	1119.7615	3039.9335	3054.0969	3081.0325
1120.7540	1125.4445	1141.7788	3101.9795	3112.6454	3186.5273
1142.1586	1142.6857	1143.3916	3188.8864	3198.0418	3204.1568
1145.5106	1146.7442	1147.0653	3210.5493	3216.0949	3218.5819
1148.2424	1150.3712	1151.0121	3223.6769	3232.1107	3245.1778
1158.8316	1161.7836	1175.6110			
1175.7125	1177.6243	1179.4400			
1180.0351	1180.9347	1183.7014			

benzaldehyde

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124.7675	221.1278	240.8417		652.3587	695.6454	712.9501
419.9719	443.3031	467.3180		718.5297	733.5171	779.9386
630.3067	662.4063	704.1124		830.6388	867.3906	872.0591
765.0632	842.6724	868.7708		938.7636	953.8052	960.1773
940.6358	983.7499	1008.0753		980.6834	985.6526	1005.1563
1018.4434	1036.9975	1051.1088		1005.9669	1017.9095	1019.5436
1110.3693	1194.1503	1199.4172		1056.0369	1058.9869	1112.0708
1234.8613	1347.6881	1370.4077		1116.6919	1173.5840	1194.4306
1441.9200	1502.5882	1539.3924		1194.4901	1210.3162	1216.1595
1642.0247	1659.6132	1800.8528		1298.8716	1349.6323	1350.4345
2907.4400	3179.2721	3189.6806		1366.5581	1368.4327	1492.4293
3201.2970	3211.5454	3221.2129		1492.9075	1536.8099	1540.1070
----				1635.2999	1636.4010	1656.9860
benzophenone				1658.3699	1739.2855	3185.3752
----				3185.5271	3195.8725	3196.2831
				3206.6770	3207.5188	3216.9198
				3220.2884	3223.8202	3224.2451
44.3327	64.6345	97.2201				
137.7430	216.0423	237.9988				
289.8185	381.1338	415.0634				
426.4442	447.9714	452.5885				

Table S5. Thermodynamics (assuming RT, in E_h) for each optimized structure.

Species	Spin	E(SCF)	H(gas)	G(gas)
<i>bis</i> -benzaldehyde	singlet	-1965.554441	-1964.176650	-1964.334403
<i>bis</i> -benzaldehyde	triplet	-1965.600742	-1964.224753	-1964.386379
<i>bis</i> -benzaldehyde	quintet	-1965.598038	-1964.222426	-1964.385495
benzaldehyde TS	triplet	-1965.591211	-1964.214461	-1964.369712
benzaldehyde diolate	triplet	-1965.630839	-1964.251098	-1964.407516
<i>bis</i> -benzophenone	singlet	-2427.667920	-2426.116132	-2426.290936
<i>bis</i> -benzophenone	triplet	-2427.718105	-2426.167170	-2426.343737
<i>bis</i> -benzophenone	quintet	-2427.716572	-2426.164857	-2426.340346
benzophenone TS	triplet	-2427.672874	-2426.123921	-2426.296175
benzophenone diolate	triplet	-2427.703287	-2426.152048	-2426.323553
<i>mono</i> -benzaldehyde	triplet	-1620.003989	-1618.748025	-1618.892187
<i>mono</i> -benzophenone	triplet	-1851.067957	-1849.725295	-1849.881179
benzaldehyde	singlet	-345.573442	-345.455984	-345.493737
benzophenone	singlet	-576.632268	-576.428567	-576.477773

8. References

1. D. F. Evans, *J. Chem. Soc.*, 1959, 2003-2005.