Electronic Supplementary Information (ESI)

Important Role of Ancillary Ligand in the Emission Behaviours of Blue-emitting Heteroleptic Ir(III) Complexes

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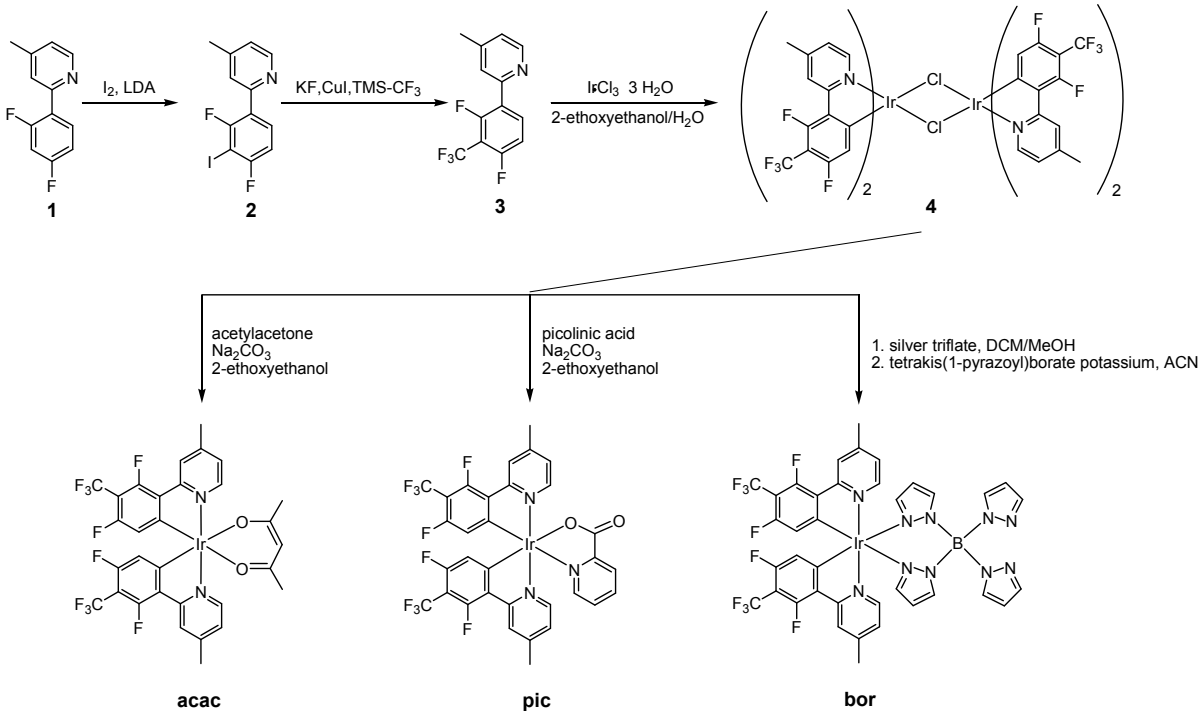

Scheme S1. Synthesis of heteroleptic Iridium(III) complexes.

EXPERIMENTAL DETAILS

General Synthetic Procedures. All preparative steps were performed under a dry nitrogen or argon atmosphere using standard Schlenk techniques. Glassware, syringes, magnetic stirring bars, and needles were dried in a convection oven for > 4 h. THF was freshly distilled over sodium/benzophenone. Other reagents were obtained commercially and used without further purification. The ligand 2-(2,4-difluoro-3-(trifluoromethyl)phenyl)-4-methylpyridine) (**3**) and cyclometalated chlorobridged diiridium(III) complex $[Ir(N^C)_2(\mu\text{-}Cl)]_2$ (**4**) were synthesized as described previously.[1] The ^1H and ^{13}C NMR spectra were recorded on a Varian Mercury 300 spectrometer operating at 300.1 and 75.4 MHz respectively. All proton and carbon chemical shifts were measured relative to internal residual benzene from the lock solvent (99.5% $CDCl_3$). The elemental analyses were

performed using a Carlo Erba Instruments CHNS-O EA 1108 analyzer, and MALDI-TOF mass spectroscopy (ABI Voyager STR) were performed by the Ochang Branches of the Korean Basic Science Institute. High Resolution Tandem Mass Spectrometry (Jeol LTD JMS-HX 110/110A) was performed at the Korean Basic Science Institute (Seoul).

Caution. *All procedures involving $IrCl_3 \bullet H_2O$ were carried out in an inert atmosphere despite the air stability of the compounds, the main concern being the oxidative and thermal stability of intermediate complexes at the high temperatures used in the reactions.*

Iridium(III) complex acac. The mixture of Ir-dimer complex **4** (0.3 g, 0.19 mmol), acetylacetone (0.04 mL, 0.37 mmol), and Na_2CO_3 (0.21 g, 1.94 mmol) was dissolved in 25 mL of 2-ethoxyethanol and refluxed for 12 h. After cooling to room temperature, the reaction mixture was poured into water. The resulting precipitate was collected by filtration and washed with water followed by *n*-hexane. The yellow powder was purified by flash column chromatography to give product as a yellow solid. Yield: 65 % (0.1 g, 0.123 mmol). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 8.24 (d, J = 5.4 Hz, 2H), 8.13 (s, 2H), 7.11 (d, J = 5.1 Hz, 2H), 5.77 (d, J = 11.1 Hz, 2H), 5.26 (s, 1H), 2.64 (s, 6H), 1.81 (s, 6H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 163.6, 160.2, 158.2, 157.0, 156.3, 150.6, 147.5, 128.4, 125.1, 124.8, 124.5, 120.9, 119.7, 31.2, 28.8, 21.9; HRMS (FAB) calcd. for $[M + H]^+$ 837.1073, Found: 837.1065; Anal. calcd for $C_{31}H_{21}F_{10}IrN_2O_2$: C, 44.55; H, 2.53; N, 3.35. Found: C, 44.50; H, 2.48; N, 3.27.

Iridium(III) complex pic. Synthesis details for **pic** were similar to those described for **acac**. The mixture of Ir-dimer complex **4** (0.3 g, 0.19 mmol), picolinic acid (0.045 g, 0.37 mmol) were reacted with Na_2CO_3 (0.06 g, 0.65 mmol) in 2-ethoxyethanol (25 mL). After cooling to room temperature, the reaction mixture was poured into water. The resulting

precipitate was collected by filtration and washed with water followed by *n*-hexane. The yellow powder was purified by flash column chromatography to give product as a yellow solid. Yield : 60% (0.097 g, 0.114 mmol). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 8.56 (d, J = 6.3 Hz, 1H), 8.34 (d, J = 7.8 Hz, 1H), 8.17 (s, 1H), 8.12 (s, 1H), 7.99 (t, J = 7.8 Hz, 1H), 7.75 (d, J = 4.5 Hz, 1H), 7.48 (t, J = 6.5 Hz, 1H), 7.25 (s, 1H), 7.10 (d, J = 6.0 Hz, 1H), 6.89 (d, J = 6.3 Hz, 1H), 5.96 (d, J = 10.8 Hz, 1H), 5.69 (d, J = 10.5 Hz, 1H), 2.58 (s, 6H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 172.6, 164.1, 162.6, 161.4, 161.0, 159.4, 157.7, 156.9, 155.8, 151.3, 148.1, 147.5, 138.9, 129.4, 128.8, 124.7, 120.8, 115.9, 21.7; HRMS (FAB) calcd. for $[M]^+$ 859.0869, Found: 859.0873; Anal. calcd for $C_{32}H_{18}F_{10}IrN_3O_2$: C, 44.76; H, 2.11; F, 22.12; Ir, 22.38; N, 4.89; O, 3.73. Found: C, 44.73; H, 2.14; N, 4.85.

Iridium(III) complex bor. The mixture of Ir dimer complex **4** (0.4 g, 0.26 mmol), silver trifluoromethanesulfonate ($AgSO_3CF_3$, 0.13 g, 0.49 mmol) was dissolved in 20 mL solution of dichloromethane: MeOH (v:v = 1:1) and stirred at room temperature for 2 h. The solution was filtered using a cannula to remove salts, the filtrate was concentrated under reduced pressure. The residue was dissolved in 20 mL of acetonitrile and added tetrakis(1-pyrazolyl)borate potassium (0.25 g, 0.78 mmol). The reaction mixture was heated to reflux at 150 ^{o}C for 12 h under nitrogen. The reaction mixture was cooled down to room temperature; then, the crude product was extracted with dichloromethane and washed with water. The combined organic layers were dried over anhydrous $MgSO_4$ and filtered. The filtrates were dried under reduced pressure and subjected to silica gel flash chromatography to give the product as a yellow solid. Yield: 25% (0.07 g, 0.065 mmol). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 8.05 (s, 2H), 7.71 (s, 2H), 7.16 (d, J = 2.4 Hz, 2H), 7.08 (d, J = 5.7 Hz, 2H), 6.88 (s, 2H), 6.65 (d, J = 5.1 Hz, 2H), 6.27 (s, 2H), 6.18 (s, 2H), 6.05 (s, 2H), 5.72 (d, J = 10.8 Hz, 2H), 2.50 (s, 6H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 162.1, 161.2, 159.5, 159.2,

157.6, 155.6, 150.0, 149.2, 144.06, 142.4, 139.2, 133.7, 129.8, 124.6, 115.5, 115.3, 107.6, 105.9, 21.6; HRMS (FAB) calcd. for $[M + H]^+$ 1017.1905, found: 1017.1920; Anal. calcd for $C_{38}H_{26}BF_{10}IrN_{10}$: C, 44.94; H, 2.58; N, 13.79. Found: C, 44.97; H, 2.56; N, 13.74.

Computational Details. Calculations used for determining the deactivation profiles were carried out using density functional theory[2,3] as implemented in the Jaguar 7.7 suite of *ab initio* quantum chemistry programs.[4] Geometry optimizations were performed with the B3LYP/6-31G** level of theory[5–8] with iridium represented by the Los Alamos LACVP basis set,[9–11] which includes relativistic effective core potentials. More reliable single point energies were computed from the optimized geometries using Dunning's correlation-consistent triple-ζ basis set, cc-pVTZ(-f),[12] where iridium was represented using a modified version of LACVP, designated as LACV3P with decontracted exponents to match the effective core potential with a triple-ζ quality basis. Vibrational frequency analysis was performed at the B3LYP/6-31G** level of theory to derive zero point energy and vibrational entropy corrections from unscaled frequencies. Entropy here refers specifically to the vibrational/rotational/translational entropy of the solute(s) as the dielectric continuum model includes the entropy of the solvent. All intermediates were confirmed to be minima on the potential energy surface possessing zero imaginary frequencies and all transition states were confirmed as saddle points by the presence of only one imaginary frequency. Solvation energies were calculated at the gas-phase optimized geometries at the double-ζ level using a dielectric constant, ε, for the dielectric continuum that represents the solvent of the experimental conditions (ε = 8.93 for dichloromethane). Solvation calculations were done at the double-ζ level using a self-consistent reaction field approach[13–15] based on accurate numerical solutions of the Poisson-Boltzmann equation.[16] As with all continuum models, the solvation energies are subject to empirical parameterization of the atomic radii

that are used to generate the solute surface. We employed the standard set of optimized radii in Jaguar for B (2.042 Å), C (1.900 Å), F (1.736 Å), H (1.150 Å), Ir (1.420 Å), N (1.600 Å), and O (1.600 Å).[15] The energy components have been computed with the following protocol. The free energy in solution phase ΔG(Sol) has been calculated as follows:

$$\Delta G(\text{Sol}) = \Delta G(\text{gas}) + \Delta G^{\text{solv}} \quad (1)$$

$$\Delta G(\text{gas}) = \Delta H(\text{gas}) - T\Delta S(\text{gas}) \quad (2)$$

$$\Delta H(\text{gas}) = \Delta E(\text{SCF}) + \Delta ZPE + \Delta C_V T + \Delta PV \quad (3)$$

$$\Delta H(\text{gas}) \approx \Delta E(\text{SCF}) + \Delta ZPE \quad (4)$$

G(gas) is the free energy in gas phase; H(gas) is the enthalpy in gas phase; T is the temperature (298 K); S(gas) is the entropy in gas phase; E(SCF) is the self-consistent field energy, i.e. "raw" electronic energy as computed from the SCF procedure and ZPE is the zero point energy. As the last two terms in equation 3 are negligibly small, this equation can be essentially reduced to equation 4. Calculations for spectra analysis and excited state evaluations were performed with the Gaussian 09 package. The characterization of the low-lying excited singlet states relies on the time-dependent DFT (TDDFT) calculations[18-23] performed at the ground-state geometry using B3LYP/LanL2DZ/6-31G** basis set.[9–12]

Crystal Structure Determination. Single crystals of **acac**, **pic** and **bor** were sealed in glass capillaries under argon and mounted on the diffractometer. The preliminary examination and data collection were performed on a Bruker SMART CCD detector system single-crystal X-ray diffractometer equipped with a sealed-tube X-ray source (50 kV × 30 mA) using graphite-monochromated Mo Kα radiation (= 0.71073 Å). The preliminary unit cell constants were determined using a set of 45 narrow-frame (0.3° in ω) scans. A double-pass

method of scanning was used to exclude any noise. The collected frames were integrated using an orientation matrix determined from the narrow-frame scans. The SMART software package was used for data collection and SAINT was used for frame integration.[24] Final cell constants were determined by a global refinement of the *xyz* centroids of the reflections harvested from the entire data set. Structure solution and refinement were carried out using the SHELXTL-PLUS software package.[25,26]

Absorption and Phosphorescence. The absorption and photoluminescence spectra were recorded on a Shimadzu UV-3101PC UV−vis−NIR scanning spectrophotometer and a Varian Cary Eclipse fluorescence spectrophotometer, respectively. The triplet energies were taken as the maximum of the first vibronic transition regarding the phosphorescence spectra. The samples dissolved in 2-methyl tetrahydrofuran (MTHF) were frozen in liquid nitrogen to 77 K. Phosphorescence was observed by irradiation of the samples at 355 nm using the third harmonic of a Qswitched Nd:YAG laser (Continuum, Surelite II, pulse width of 4.5 ns) combined with a homemade Raman shifter. Temporal profiles were measured by a photomultiplier (Zolix Instruments Co., CR 131) and a digital oscilloscope (Tektronix, TDS-784D) equipped with a monochromator (DongWooOptron, Monora 500i). Reported signals were obtained as averages of 500 events. The detection window was set to 15 μs, and the delay was set to 1 ms from the rigging edge of the laser.

Thermal Properties. Thermal properties were measured using differential scanning calorimetry (Perkin-Elmer/Pyris Diamond DSC). A heating rate of 10 °C/min was used after first melting the compound, followed by a rapid cooling rate of 40 °C/min to room temperature.

OLED Devices. Before device fabrication, all of the prepared Ir(III) complexes, **acac**, **pic**, and **bor** were purified by train sublimation in 51, 56, 58, and 42 % yields, respectively. The OLED devices were fabricated on glass substrates pre-coated with a 150 nm ITO layer having a sheet resistance of 10 Ω/square. The ITO glass was pre-cleaned using a conventional solvent cleaning method. The ITO surface was cleaned again with a UV ozone treatment immediately before depositing the hole transporting layer (HTL). The organic, LiF, and Al layers were deposited sequentially onto the substrate without breaking the vacuum. The current-voltage characteristics of OLEDs were measured using a source measure unit (Keithley 236). The electroluminescence spectra, luminance, and CIE coordinates were measured using a spectro-radiometer (Photo Research PR650). Assuming Lambertian emission, the external quantum efficiency (EQE) was calculated from the luminance, current density, and electroluminescence spectrum.

Table S1. Crystal data and structure refinement for compound **acac**, **pic**, and **bor**.

Identification code	**acac**	**pic**	**bor**
Empirical formula	$C_{31}H_{21}F_{10}IrN_2O_2$	$C_{30}H_{14}F_{10}IrN_3O_2$	$C_{38}H_{26}BF_{10}IrN_{10}$
Formula weight	835.70	830.66	1015.70
Temperature	293(2) K	293(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system, space group	Orthorhombic, *Pccn*	Monoclinic, $P2_1/c$	Triclinic, *P*-1
Unit cell dimensions	a = 21.281(1) Å b = 7.927(5) Å c = 17.697(1) Å	a = 12.378(7) Å b = 11.046(6) Å β = 111.24(2)° c = 25.909(1) Å	a = 10.044(4) Å α = 107.895(6)° b = 13.686(5) Å β = 96.247(7)° c = 17.345(7) Å γ = 107.337(6)°
Volume	2985.6(3) Å^3	3302.0(3) Å^3	2112.5(1) Å^3
Z, Calculated density	4, 1.859 Mg/m^3	4, 1.671 Mg/m^3	2, 1.597 Mg/m^3
μ	4.567 mm^{-1}	4.130 mm^{-1}	3.245 mm^{-1}
F(000)	1616	1592	992
Crystal size	0.25 * 0.18 * 0.12 mm	0.23 * 0.14 * 0.13 mm	0.40 * 0.14 * 0.18 mm
θ range for data collection	2.302 to 28.311°	1.950 to 28.341°	1.265 to 28.373°
Limiting indices	$-28 \le h \le 28$, $-10 \le k \le 10$, $-23 \le l \le 23$	$-16 \le h \le 16$, $-14 \le k \le 14$, $-32 \le l \le 34$	$-13 \le h \le 13$, $-18 \le k \le 18$, $-23 \le l \le 23$
Reflections collected / unique	38254 / 3719 [R_{int} = 0.0377]	26011 / 8209 [R_{int} = 0.0283]	17375 / 6943 [R_{int} = 0.0489]
Completeness to θ = 25.242	100.0%	99.9%	60.1%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Data / restraints / parameters	3719 / 0 / 212	8209 / 0 / 415	6943 / 0 / 541
Goodness-of-fit on F^2	0.983	1.084	0.985
Final R indices [$I>2\sigma(I)$]	$R_1{}^a$ = 0.0294, $wR_2{}^b$ = 0.0743	$R_1{}^a$ = 0.0471, $wR_2{}^b$ = 0.1399	$R_1{}^a$ = 0.0392, $wR_2{}^b$ = 0.0960
R indices (all data)	$R_1{}^a$ = 0.0393, $wR_2{}^b$ = 0.0821	$R_1{}^a$ = 0.0559, $wR_2{}^b$ = 0.1468	$R_1{}^a$ = 0.0476, $wR_2{}^b$ = 0.0994
Largest diff. peak and hole	2.258 and -0.740 e. Å^{-3}	6.069 and -0.781 e. Å^{-3}	1.230 and -0.803 e. Å^{-3}

$^aR_1 = \sum||F_o|-|F_c|| / \sum|F_o|$ (based on reflections with $F_o^2 > 2\sigma(F_o^2)$)

$^bwR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; $P = [\max(F_o^2, 0)+2F_c^2]/3$ (also with $F_o^2 > 2\sigma(F_o^2)$)

Table S2. Bond lengths [Å] and angles [°] for **acac**.

Bond Lengths [Å]			
Ir(1)-C(1)	1.971(3)	C(2)-C(3)	1.377(6)
Ir(1)-N(1)	2.034(3)	C(2)-C(8)	1.473(5)
Ir(1)-O(1)	2.125(3)	C(3)-C(4)	1.392(6)
F(1)-C(3)	1.352(5)	C(4)-C(5)	1.390(6)
F(2)-C(5)	1.348(5)	C(4)-C(7)	1.508(7)
F(3)-C(7)	1.274(8)	C(5)-C(6)	1.357(6)
F(4)-C(7)	1.309(9)	C(8)-C(12)	1.392(5)
F(5)-C(7)	1.223(8)	C(9)-C(10)	1.360(7)
O(1)-C(14)	1.276(5)	C(10)-C(11)	1.376(8)
N(1)-C(9)	1.344(5)	C(11)-C(12)	1.390(7)
N(1)-C(8)	1.365(5)	C(11)-C(13)	1.521(7)
C(1)-C(6)	1.398(5)	C(14)-C(15)	1.392(6)
C(1)-C(2)	1.420(5)	C(14)-C(16)	1.504(7)
Bond Angles [°]			
C(1)-Ir(1)-C(1)#1	89.6(2)	C(2)-C(3)-C(4)	123.9(4)
C(1)-Ir(1)-N(1)	80.8(1)	C(3)-C(4)-C(5)	115.0(4)
C(1)#1-Ir(1)-N(1)	95.8(1)	C(3)-C(4)-C(7)	121.8(4)
C(1)-Ir(1)-N(1)#1	95.8(1)	C(5)-C(4)-C(7)	123.2(4)
C(1)#1-Ir(1)-N(1)#1	80.8(1)	F(2)-C(5)-C(6)	118.0(4)
N(1)-Ir(1)-N(1)#1	175.3(2)	F(2)-C(5)-C(4)	118.3(4)
C(1)-Ir(1)-O(1)	90.8(1)	C(6)-C(5)-C(4)	123.7(4)
C(1)#1-Ir(1)-O(1)	175.6(1)	C(5)-C(6)-C(1)	120.8(4)
N(1)-Ir(1)-O(1)	88.6(1)	F(5)-C(7)-F(3)	109.4(7)
N(1)#1-Ir(1)-O(1)	94.8(1)	F(5)-C(7)-F(4)	105.5(7)
C(1)-Ir(1)-O(1)#1	175.6(1)	F(3)-C(7)-F(4)	100.4(7)
C(1)#1-Ir(1)-O(1)#1	90.8(1)	F(5)-C(7)-C(4)	115.9(5)
N(1)-Ir(1)-O(1)#1	94.8(1)	F(3)-C(7)-C(4)	113.0(6)
N(1)#1-Ir(1)-O(1)#1	88.6(1)	F(4)-C(7)-C(4)	111.4(6)
O(1)-Ir(1)-O(1)#1	89.2(2)	N(1)-C(8)-C(12)	119.7(4)
C(14)-O(1)-Ir(1)	124.6(3)	N(1)-C(8)-C(2)	112.4(3)

C(9)-N(1)-C(8)	119.1(4)	C(12)-C(8)-C(2)	127.9(4)
C(9)-N(1)-Ir(1)	124.2(3)	N(1)-C(9)-C(10)	122.7(5)
C(8)-N(1)-Ir(1)	116.7(2)	C(9)-C(10)-C(11)	120.0(5)
C(6)-C(1)-C(2)	117.5(3)	C(10)-C(11)-C(12)	118.0(4)
C(6)-C(1)-Ir(1)	127.6(3)	C(10)-C(11)-C(13)	121.6(5)
C(2)-C(1)-Ir(1)	114.9(3)	C(12)-C(11)-C(13)	120.4(6)
C(3)-C(2)-C(1)	119.1(3)	C(11)-C(12)-C(8)	120.6(5)
C(3)-C(2)-C(8)	125.7(4)	O(1)-C(14)-C(15)	126.8(5)
C(1)-C(2)-C(8)	115.2(3)	O(1)-C(14)-C(16)	114.4(5)
F(1)-C(3)-C(2)	119.7(4)	C(15)-C(14)-C(16)	118.8(5)
F(1)-C(3)-C(4)	116.4(4)	C(14)-C(15)-C(14)#1	128.1(6)

Symmetry transformations used to generate equivalent atoms:
1 -x+1/2, -y+3/2, z

Table S3. Bond lengths [Å] and angles [°] for **pic**.

Bond Lengths [Å]			
O(1)-C(32)	1.285(5)	C(3)-C(4)	1.383(6)
O(1)-Ir(1)	2.140(3)	C(4)-C(5)	1.378(6)
O(2)-C(32)	1.212(5)	C(4)-C(7)	1.489(7)
N(2)-C(21)	1.352(5)	C(5)-C(6)	1.361(6)
N(2)-C(22)	1.355(5)	C(8)-C(12)	1.374(5)
N(2)-Ir(1)	2.032(3)	C(9)-C(10)	1.371(6)
N(1)-C(9)	1.335(5)	C(10)-C(11)	1.374(6)
N(1)-C(8)	1.372(4)	C(11)-C(12)	1.396(5)
N(1)-Ir(1)	2.053(3)	C(11)-C(13)	1.484(6)
N(3)-C(31)	1.336(5)	C(14)-C(19)	1.407(5)
N(3)-C(27)	1.349(5)	C(14)-C(15)	1.434(5)
N(3)-Ir(1)	2.143(3)	C(15)-C(16)	1.376(6)
Ir(1)-C(14)	1.980(4)	C(15)-C(21)	1.479(5)
Ir(1)-C(1)	2.003(4)	C(16)-C(17)	1.391(6)
F(1)-C(3)	1.344(5)	C(17)-C(18)	1.389(6)
F(2)-C(5)	1.362(5)	C(17)-C(20)	1.502(6)
F(3)-C(7)	1.235(7)	C(18)-C(19)	1.371(6)
F(4)-C(7)	1.280(1)	C(21)-C(25)	1.390(5)
F(5)-C(7)	1.230(9)	C(22)-C(23)	1.359(6)
F(6)-C(16)	1.350(4)	C(23)-C(24)	1.385(6)
F(7)-C(18)	1.356(5)	C(24)-C(25)	1.418(6)
F(8)-C(20)	1.335(7)	C(24)-C(26)	1.500(6)
F(9)-C(20)	1.303(6)	C(27)-C(28)	1.391(7)
F(10)-C(20)	1.313(6)	C(28)-C(29)	1.347(8)
C(1)-C(6)	1.391(6)	C(29)-C(30)	1.398(8)
C(1)-C(2)	1.414(5)	C(30)-C(31)	1.387(6)
C(2)-C(3)	1.380(5)	C(31)-C(32)	1.516(6)
C(2)-C(8)	1.477(5)		
Bond Angles [°]			
C(32)-O(1)-Ir(1)	117.2(2)	C(12)-C(8)-C(2)	128.2(3)

C(21)-N(2)-C(22)	118.8(3)	N(1)-C(9)-C(10)	123.0(4)
C(21)-N(2)-Ir(1)	117.0(2)	C(9)-C(10)-C(11)	120.6(4)
C(22)-N(2)-Ir(1)	124.2(3)	C(10)-C(11)-C(12)	116.0(4)
C(9)-N(1)-C(8)	118.5(3)	C(10)-C(11)-C(13)	122.1(4)
C(9)-N(1)-Ir(1)	125.1(3)	C(12)-C(11)-C(13)	121.9(4)
C(8)-N(1)-Ir(1)	116.4(2)	C(8)-C(12)-C(11)	122.4(4)
C(31)-N(3)-C(27)	119.2(4)	C(19)-C(14)-C(15)	117.4(3)
C(31)-N(3)-Ir(1)	113.9(3)	C(19)-C(14)-Ir(1)	128.5(3)
C(27)-N(3)-Ir(1)	126.4(3)	C(15)-C(14)-Ir(1)	114.1(3)
C(14)-Ir(1)-C(1)	90.7(2)	C(16)-C(15)-C(14)	119.1(3)
C(14)-Ir(1)-N(2)	80.8(1)	C(16)-C(15)-C(21)	126.1(3)
C(1)-Ir(1)-N(2)	96.2(1)	C(14)-C(15)-C(21)	114.8(3)
C(14)-Ir(1)-N(1)	97.1(1)	F(6)-C(16)-C(15)	119.9(4)
C(1)-Ir(1)-N(1)	80.7(1)	F(6)-C(16)-C(17)	116.1(4)
N(2)-Ir(1)-N(1)	176.2(1)	C(15)-C(16)-C(17)	124.0(4)
C(14)-Ir(1)-O(1)	171.1(1)	C(18)-C(17)-C(16)	115.5(4)
C(1)-Ir(1)-O(1)	95.8(1)	C(18)-C(17)-C(20)	125.3(4)
N(2)-Ir(1)-O(1)	92.4(1)	C(16)-C(17)-C(20)	119.2(4)
N(1)-Ir(1)-O(1)	90.1(1)	F(7)-C(18)-C(19)	117.0(4)
C(14)-Ir(1)-N(3)	97.3(1)	F(7)-C(18)-C(17)	119.4(4)
C(1)-Ir(1)-N(3)	170.6(1)	C(19)-C(18)-C(17)	123.6(4)
N(2)-Ir(1)-N(3)	90.1(1)	C(18)-C(19)-C(14)	120.4(4)
N(1)-Ir(1)-N(3)	93.2(1)	F(9)-C(20)-F(10)	109.7(5)
O(1)-Ir(1)-N(3)	76.9(1)	F(9)-C(20)-F(8)	103.6(5)
C(6)-C(1)-C(2)	118.0(3)	F(10)-C(20)-F(8)	103.9(4)
C(6)-C(1)-Ir(1)	127.9(3)	F(9)-C(20)-C(17)	113.8(4)
C(2)-C(1)-Ir(1)	114.1(3)	F(10)-C(20)-C(17)	114.0(4)
C(3)-C(2)-C(1)	119.0(4)	F(8)-C(20)-C(17)	110.9(4)
C(3)-C(2)-C(8)	124.6(4)	N(2)-C(21)-C(25)	121.4(3)
C(1)-C(2)-C(8)	116.4(3)	N(2)-C(21)-C(15)	112.5(3)
F(1)-C(3)-C(2)	120.0(4)	C(25)-C(21)-C(15)	126.1(3)
F(1)-C(3)-C(4)	116.6(4)	N(2)-C(22)-C(23)	121.9(4)

C(2)-C(3)-C(4)	123.4(4)	C(22)-C(23)-C(24)	121.5(4)
C(5)-C(4)-C(3)	115.3(4)	C(23)-C(24)-C(25)	116.5(4)
C(5)-C(4)-C(7)	123.6(4)	C(23)-C(24)-C(26)	123.2(5)
C(3)-C(4)-C(7)	121.0(5)	C(25)-C(24)-C(26)	120.3(5)
C(6)-C(5)-F(2)	117.7(4)	C(21)-C(25)-C(24)	119.7(4)
C(6)-C(5)-C(4)	124.2(4)	N(3)-C(27)-C(28)	120.8(5)
F(2)-C(5)-C(4)	118.1(4)	C(29)-C(28)-C(27)	120.1(5)
C(5)-C(6)-C(1)	119.9(4)	C(28)-C(29)-C(30)	119.7(5)
F(5)-C(7)-F(3)	105.2(8)	C(31)-C(30)-C(29)	117.8(5)
F(5)-C(7)-F(4)	103.3(8)	N(3)-C(31)-C(30)	122.3(4)
F(3)-C(7)-F(4)	101.8(8)	N(3)-C(31)-C(32)	116.8(3)
F(5)-C(7)-C(4)	114.7(6)	C(30)-C(31)-C(32)	120.9(4)
F(3)-C(7)-C(4)	118.6(5)	O(2)-C(32)-O(1)	125.7(4)
F(4)-C(7)-C(4)	111.6(6)	O(2)-C(32)-C(31)	119.7(4)
N(1)-C(8)-C(12)	119.5(3)	O(1)-C(32)-C(31)	114.6(3)
N(1)-C(8)-C(2)	112.3(3)		

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond lengths [Å] and angles [°] for **bor**.

Bond Lengths [Å]			
Ir(1)-C(20)	2.002(5)	C(1)-C(2)	1.345(1)
Ir(1)-C(7)	2.008(4)	C(2)-C(3)	1.381(1)
Ir(1)-N(1)	2.047(5)	C(3)-C(4)	1.372(1)
Ir(1)-N(2)	2.051(5)	C(3)-C(12)	1.507(1)
Ir(1)-N(3)	2.133(4)	C(4)-C(5)	1.396(1)
Ir(1)-N(5)	2.143(5)	C(5)-C(6)	1.482(8)
F(1)-C(9)	1.350(7)	C(6)-C(11)	1.382(8)
F(2)-C(11)	1.339(9)	C(6)-C(7)	1.407(8)
F(3)-C(13)	1.410(2)	C(7)-C(8)	1.383(7)
F(5)-C(13)	1.177(2)	C(8)-C(9)	1.388(7)
F(6)-C(22)	1.363(7)	C(9)-C(10)	1.355(1)
F(7)-C(24)	1.342(8)	C(10)-C(11)	1.403(1)
F(8)-C(26)	1.316(1)	C(10)-C(13)	1.504(9)
F(9)-C(26)	1.286(1)	C(13)-F(4)	1.264(2)
F(10)-C(26)	1.289(1)	C(14)-C(15)	1.388(9)
N(1)-C(1)	1.351(7)	C(15)-C(16)	1.380(1)
N(1)-C(5)	1.380(7)	C(16)-C(17)	1.393(9)
N(2)-C(14)	1.337(7)	C(16)-C(25)	1.495(1)
N(2)-C(18)	1.374(7)	C(17)-C(18)	1.401(9)
N(3)-C(29)	1.336(7)	C(18)-C(19)	1.483(7)
N(3)-N(4)	1.369(7)	C(19)-C(20)	1.392(8)
N(4)-C(27)	1.355(7)	C(19)-C(24)	1.403(9)
N(4)-B(1)	1.521(8)	C(20)-C(21)	1.402(7)
N(5)-C(32)	1.343(6)	C(21)-C(22)	1.369(9)
N(5)-N(6)	1.351(7)	C(22)-C(23)	1.368(1)
N(6)-C(30)	1.357(8)	C(23)-C(24)	1.401(8)
N(6)-B(1)	1.548(7)	C(23)-C(26)	1.508(1)
N(7)-N(8)	1.350(1)	C(27)-C(28)	1.360(1)
N(7)-C(35)	1.369(1)	C(28)-C(29)	1.386(9)
N(7)-B(1)	1.553(8)	C(30)-C(31)	1.338(9)

N(8)-C(33)	1.402(2)	C(31)-C(32)	1.384(1)
N(9)-N(10)	1.371(8)	C(33)-C(34)	1.315(2)
N(9)-C(38)	1.379(9)	C(34)-C(35)	1.304(1)
N(9)-B(1)	1.528(1)	C(36)-C(37)	1.376(2)
N(10)-C(36)	1.314(1)	C(37)-C(38)	1.331(2)

Bond Angles [°]			
C(20)-Ir(1)-C(7)	87.3(2)	C(9)-C(10)-C(13)	123.2(8)
C(20)-Ir(1)-N(1)	95.6(2)	C(11)-C(10)-C(13)	120.5(8)
C(7)-Ir(1)-N(1)	80.6(2)	F(2)-C(11)-C(6)	120.8(6)
C(20)-Ir(1)-N(2)	80.6(2)	F(2)-C(11)-C(10)	116.9(5)
C(7)-Ir(1)-N(2)	96.3(2)	C(6)-C(11)-C(10)	122.2(6)
N(1)-Ir(1)-N(2)	175.2(2)	F(5)-C(13)-F(4)	116.3(1)
C(20)-Ir(1)-N(3)	92.8(2)	F(5)-C(13)-F(3)	103.2(1)
C(7)-Ir(1)-N(3)	175.7(2)	F(4)-C(13)-F(3)	88.1(1)
N(1)-Ir(1)-N(3)	95.1(2)	F(5)-C(13)-C(10)	117.7(1)
N(2)-Ir(1)-N(3)	88.0(2)	F(4)-C(13)-C(10)	116.0(1)
C(20)-Ir(1)-N(5)	173.7(2)	F(3)-C(13)-C(10)	110.0(1)
C(7)-Ir(1)-N(5)	91.1(2)	N(2)-C(14)-C(15)	123.1(6)
N(1)-Ir(1)-N(5)	90.2(2)	C(16)-C(15)-C(14)	120.2(6)
N(2)-Ir(1)-N(5)	93.6(2)	C(15)-C(16)-C(17)	117.3(7)
N(3)-Ir(1)-N(5)	89.3(2)	C(15)-C(16)-C(25)	122.1(7)
C(1)-N(1)-C(5)	117.9(6)	C(17)-C(16)-C(25)	120.6(8)
C(1)-N(1)-Ir(1)	125.4(4)	C(16)-C(17)-C(18)	120.6(7)
C(5)-N(1)-Ir(1)	116.7(4)	N(2)-C(18)-C(17)	120.7(5)
C(14)-N(2)-C(18)	118.0(5)	N(2)-C(18)-C(19)	112.0(5)
C(14)-N(2)-Ir(1)	125.7(4)	C(17)-C(18)-C(19)	127.2(5)
C(18)-N(2)-Ir(1)	116.2(3)	C(20)-C(19)-C(24)	120.7(5)
C(29)-N(3)-N(4)	106.5(4)	C(20)-C(19)-C(18)	116.4(5)
C(29)-N(3)-Ir(1)	126.6(4)	C(24)-C(19)-C(18)	122.9(6)
N(4)-N(3)-Ir(1)	126.8(3)	C(19)-C(20)-C(21)	118.0(5)
C(27)-N(4)-N(3)	107.8(5)	C(19)-C(20)-Ir(1)	114.6(4)

C(27)-N(4)-B(1)	125.9(5)	C(21)-C(20)-Ir(1)	127.3(4)
N(3)-N(4)-B(1)	125.1(4)	C(22)-C(21)-C(20)	120.1(6)
C(32)-N(5)-N(6)	106.4(5)	F(6)-C(22)-C(23)	118.5(6)
C(32)-N(5)-Ir(1)	126.1(4)	F(6)-C(22)-C(21)	118.3(6)
N(6)-N(5)-Ir(1)	124.6(3)	C(23)-C(22)-C(21)	123.2(5)
N(5)-N(6)-C(30)	108.9(4)	C(22)-C(23)-C(24)	117.5(6)
N(5)-N(6)-B(1)	123.2(5)	C(22)-C(23)-C(26)	121.2(6)
C(30)-N(6)-B(1)	125.2(5)	C(24)-C(23)-C(26)	121.3(7)
N(8)-N(7)-C(35)	111.1(7)	F(7)-C(24)-C(23)	119.0(6)
N(8)-N(7)-B(1)	128.9(8)	F(7)-C(24)-C(19)	120.5(5)
C(35)-N(7)-B(1)	120.0(6)	C(23)-C(24)-C(19)	120.4(6)
N(7)-N(8)-C(33)	104.2(1)	F(9)-C(26)-F(10)	103.2(9)
N(10)-N(9)-C(38)	109.0(7)	F(9)-C(26)-F(8)	105.2(9)
N(10)-N(9)-B(1)	121.0(5)	F(10)-C(26)-F(8)	105.5(8)
C(38)-N(9)-B(1)	129.5(6)	F(9)-C(26)-C(23)	112.4(8)
C(36)-N(10)-N(9)	104.9(7)	F(10)-C(26)-C(23)	113.1(7)
C(2)-C(1)-N(1)	122.8(6)	F(8)-C(26)-C(23)	116.3(6)
C(1)-C(2)-C(3)	120.9(6)	N(4)-C(27)-C(28)	110.3(6)
C(4)-C(3)-C(2)	117.5(8)	C(27)-C(28)-C(29)	104.0(5)
C(4)-C(3)-C(12)	120.5(8)	N(3)-C(29)-C(28)	111.2(6)
C(2)-C(3)-C(12)	122.0(7)	C(31)-C(30)-N(6)	109.0(6)
C(3)-C(4)-C(5)	120.9(7)	C(30)-C(31)-C(32)	105.8(5)
N(1)-C(5)-C(4)	119.8(5)	N(5)-C(32)-C(31)	109.8(5)
N(1)-C(5)-C(6)	111.7(6)	C(34)-C(33)-N(8)	106.9(8)
C(4)-C(5)-C(6)	128.3(5)	C(35)-C(34)-C(33)	113.3(1)
C(11)-C(6)-C(7)	119.5(5)	C(34)-C(35)-N(7)	104.6(8)
C(11)-C(6)-C(5)	124.0(6)	N(10)-C(36)-C(37)	112.4(9)
C(7)-C(6)-C(5)	116.6(5)	C(38)-C(37)-C(36)	105.7(9)
C(8)-C(7)-C(6)	118.7(4)	C(37)-C(38)-N(9)	107.9(8)
C(8)-C(7)-Ir(1)	127.2(4)	N(4)-B(1)-N(9)	111.3(5)
C(6)-C(7)-Ir(1)	114.1(4)	N(4)-B(1)-N(6)	113.5(5)
C(7)-C(8)-C(9)	119.4(6)	N(9)-B(1)-N(6)	108.0(4)

F(1)-C(9)-C(10)	119.1(5)	N(4)-B(1)-N(7)	108.1(4)
F(1)-C(9)-C(8)	117.1(6)	N(9)-B(1)-N(7)	107.8(5)
C(10)-C(9)-C(8)	123.8(6)	N(6)-B(1)-N(7)	107.9(5)
C(9)-C(10)-C(11)	116.3(5)		

Symmetry transformations used to generate equivalent atoms:

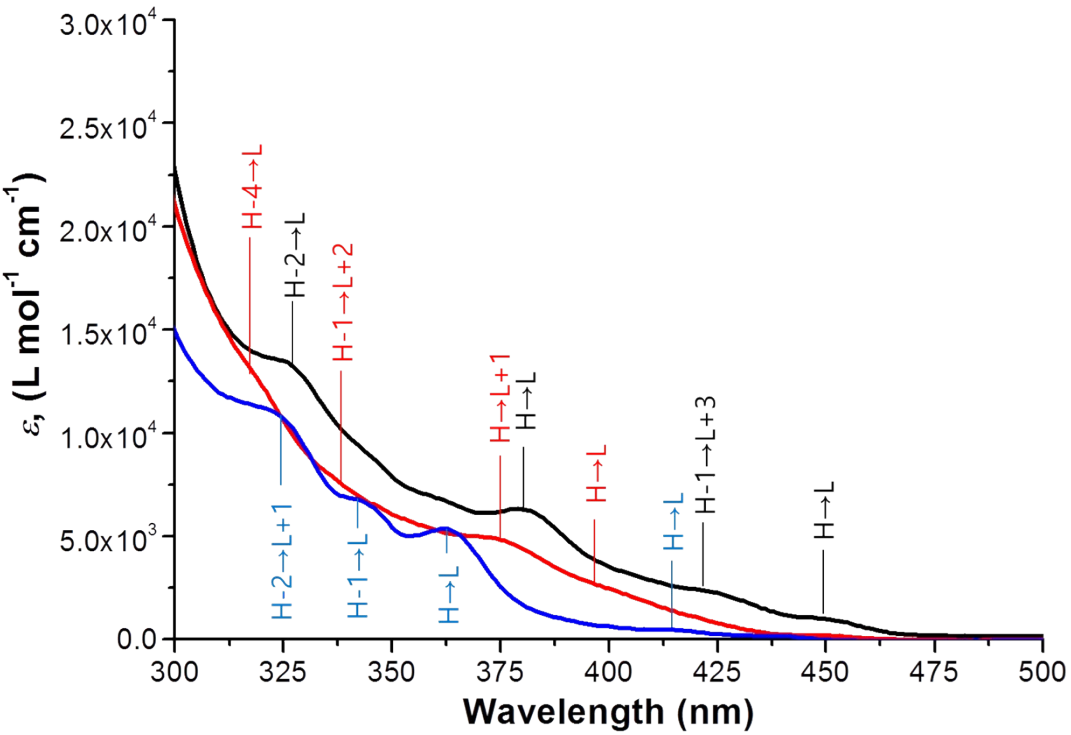

Fig. S1 Experimental absorption spectra and calculated singlet transition for **acac** (black), **pic** (red) and **bor** (blue).

Table S5. Energy levels of the lower lying transitions of complex **acac**, **pic** and **bor** calculated from the TDDFT approach.

	State	assgnt	λ (nm)	(*f*)
acac	S	HOMO→LUMO+2 (28%), HOMO-2→LUMO (60%)	324.0	0.0611
	S	HOMO-1→LUMO+1 (95%)	368.6	0.0448
	S	HOMO→LUMO (96%)	396.9	0.0366
	T	HOMO→LUMO (61%), HOMO-3→LUMO+1 (14%)	436.8	-
pic	S	HOMO-4→LUMO+2 (48%), HOMO-4→LUMO (17%)	313.8	0.0206
	S	HOMO-4→LUMO (46%), HOMO→LUMO+4 (34%)	319.6	0.0253
	S	HOMO-1→LUMO+2 (72%), HOMO→LUMO+3 (14%)	339.2	0.0374
	S	HOMO→LUMO+1 (90%)	386.1	0.0025
	S	HOMO→LUMO (87%)	396.7	0.0286
	T	HOMO→LUMO (56%), HOMO-4→LUMO (12%)	435.6	-
bor	S	HOMO-3→LUMO+1 (65%), HOMO-1→LUMO+1 (17%)	320.1	0.0227
	S	HOMO-2→LUMO+1 (45%), HOMO-3→LUMO (19%)	329.4	0.0712
	S	HOMO-1→LUMO (26%), HOMO-2→LUMO+1 (23%)	335.2	0.0256
	S	HOMO→LUMO (96%)	366.6	0.0106
	T	HOMO→LUMO (46%), HOMO-6→LUMO (10%)	423.7	-

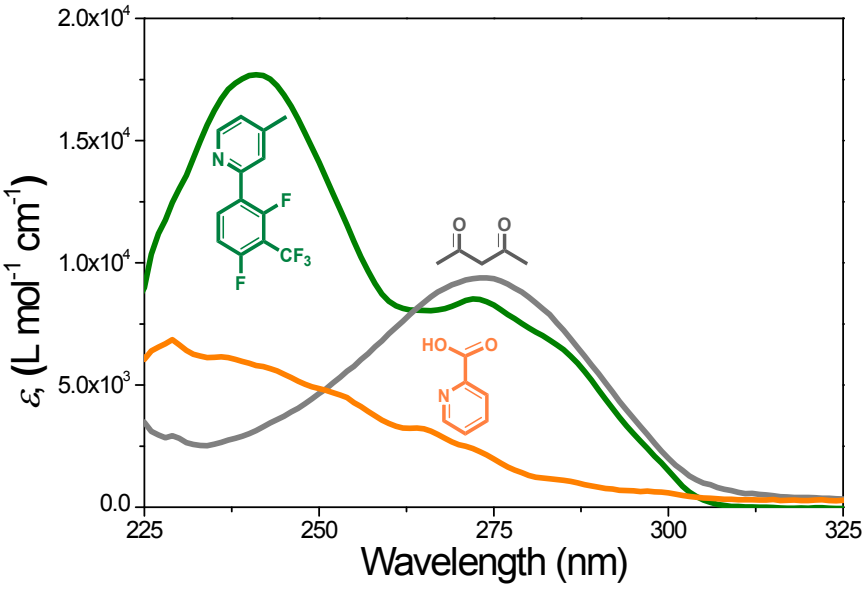

Fig. S2 Experimental absorption spectra for dfCF_3, acac, and pic ligand in dichloromethane solution at room temperature.

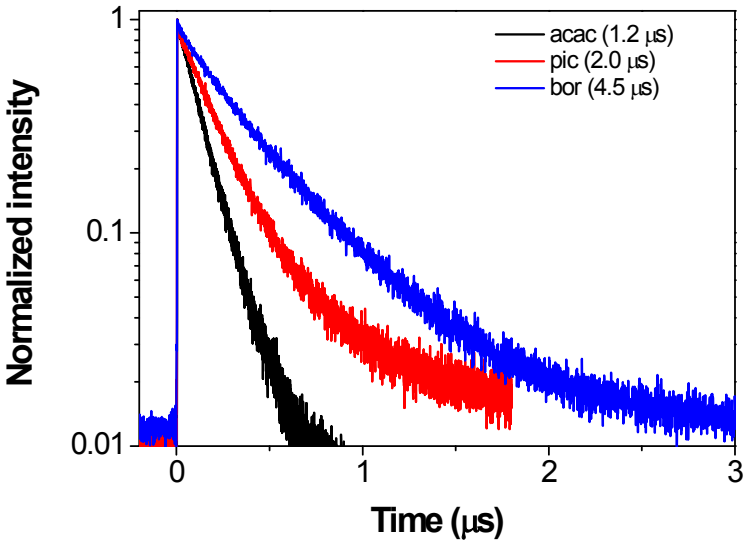

Fig. S3 Emission decay profiles for **acac, pic** and **bor** in PMMA films (0.5wt%).

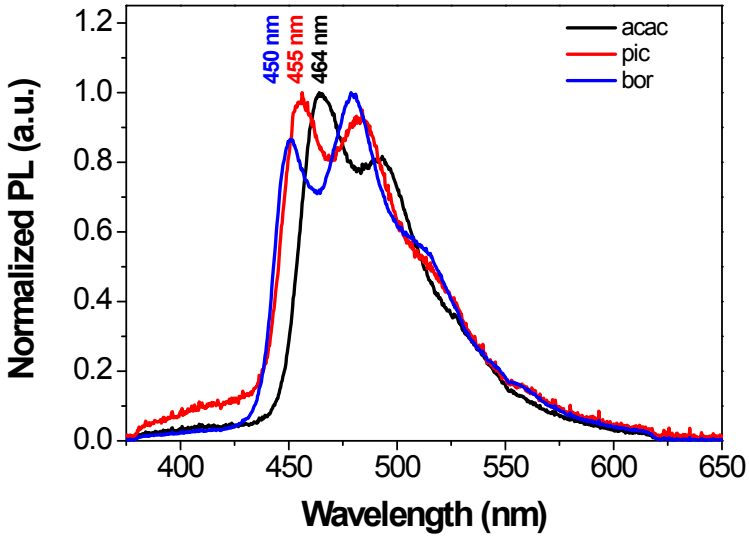

Fig. S4 Emission spectra for **acac, pic** and **bor** in PMMA films (0.5wt%).

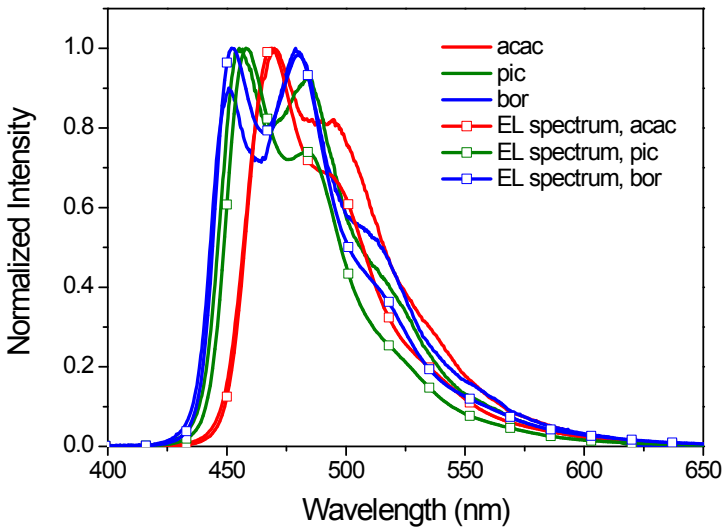

Fig. S5 Emission spectra of Ir complexes and the electroluminescent (EL) spectra.

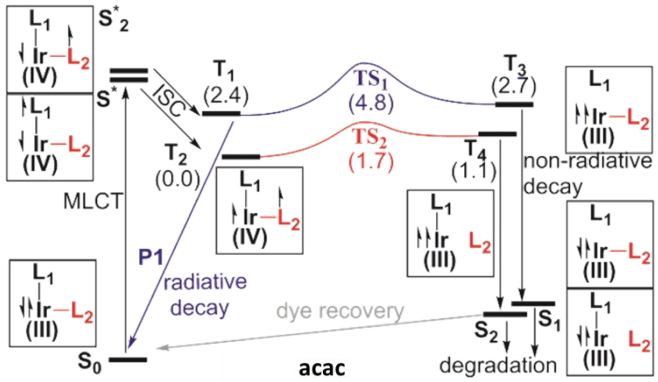

Fig. S6 Reaction profile for Ir–ligand bond cleavage to form non-radiative $\mathbf{T_3}$ and $\mathbf{T_4}$ states for **acac**.

Fig. S5 shows the reaction profile for the generation of the non-radiative intermediates for **acac**. Our calculations suggest that the T_2 state, where the electron is excited in to the acac ligand is actually 2.3 kcal mol^{-1} lower in energy than the T_1 state with the electron promoted into the cyclometalating $dfCF_3$ ligand. In the $\mathbf{T_2}$ state, there is a Mulliken spin density of 0.292 on Ir and of 1.654 distributed across the acac moiety. The $\mathbf{T_3}$ state is nearly isoenergetic with the $\mathbf{T_1}$ state and the barrier $\mathbf{TS_1}$ to cleave the Ir–pyridine bond is only 4.8 kcal mol^{-1} in reference to the lowest energy $\mathbf{T_2}$ state and just 2.5 kcal mol^{-1} from the $\mathbf{T_1}$ state. This barrier is consistent with the experimental result that **acac** exhibits a significantly shorter photoluminescence lifetime and increased non-radiative decay rates. This low-lying π^*-orbitals of $\mathbf{T_2}$ state may interfere with populating the desired $\mathbf{T_1}$ state and can also potentially undergo a similar metal ligand bond cleavage deactivation mechanism to reach the $\mathbf{T_4}$ state, which is 1.1 kcal mol^{-1} thermodynamically higher in energy than the $\mathbf{T_2}$ state. At the $\mathbf{T_4}$ state the Ir–O bond distance has lengthened to and 2.664 Å from 2.120 Å. The kinetic barrier $\mathbf{TS_2}$ to overcome to reach the $\mathbf{T_4}$ state is only 1.7 kcal mol^{-1} providing another readily accessible route to non-radiative decay. At the transition state, the Ir–O bond distance has increased to 2.384 Å and the Mulliken spin density has increased to 0.920 compared to 1.101 in the $\mathbf{T_4}$ state. Even though the calculated absolute values could be different with experimental values, we believe that the tendency of calculated results can support experimental data. We expect that these accessible non-radiative states should be responsible for the decreased lifetime of **acac** seen experimentally.

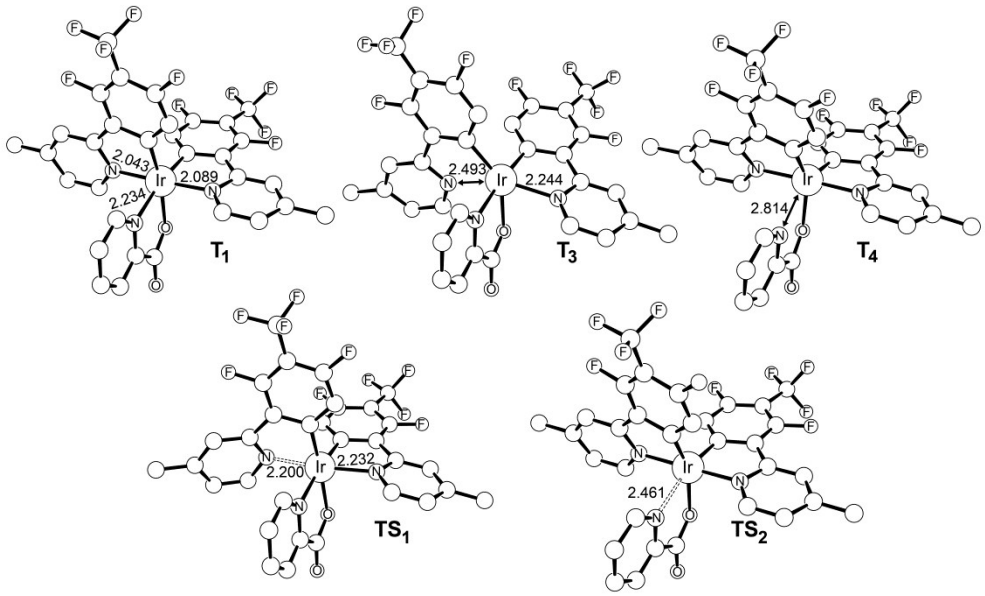

Fig. S7 Optimized structures of $\mathbf{T_1}$, $\mathbf{T_3}$, $\mathbf{T_4}$ states and transition states $\mathbf{TS_1}$ and $\mathbf{TS_2}$ for **pic**.

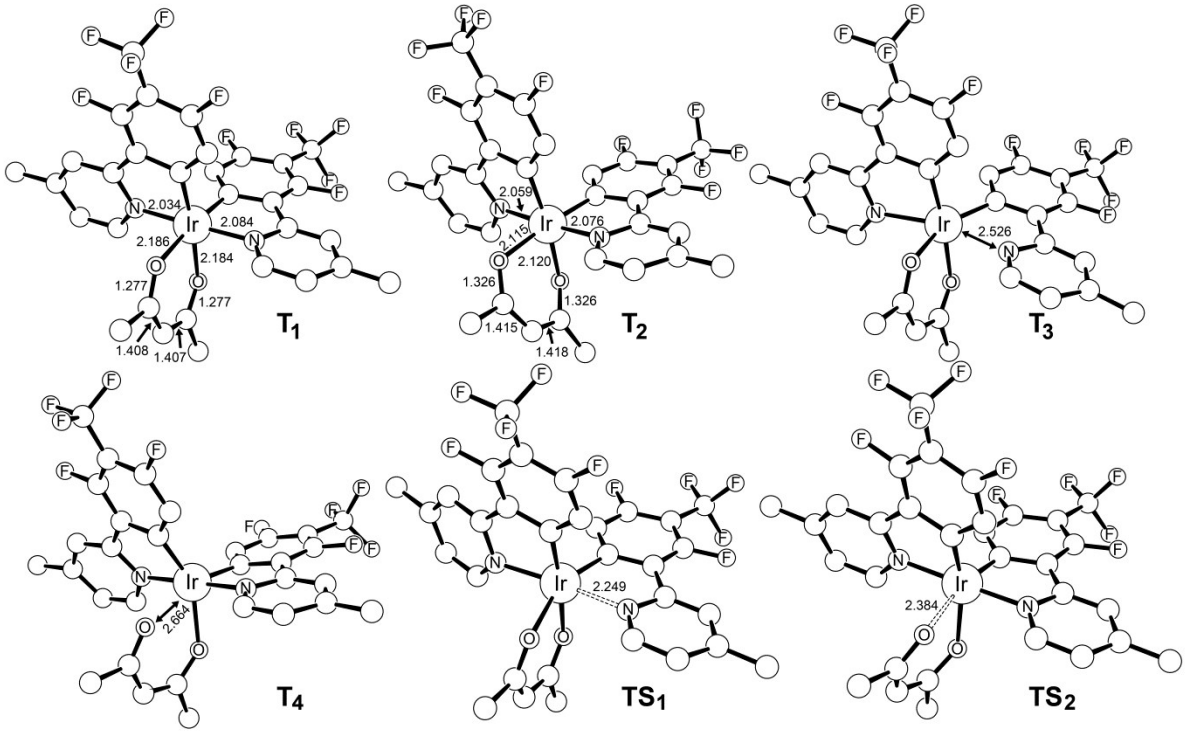

Fig. S8 Optimized structures of triplet states and transition states $\mathbf{TS_1}$ and $\mathbf{TS_2}$ for **acac**.

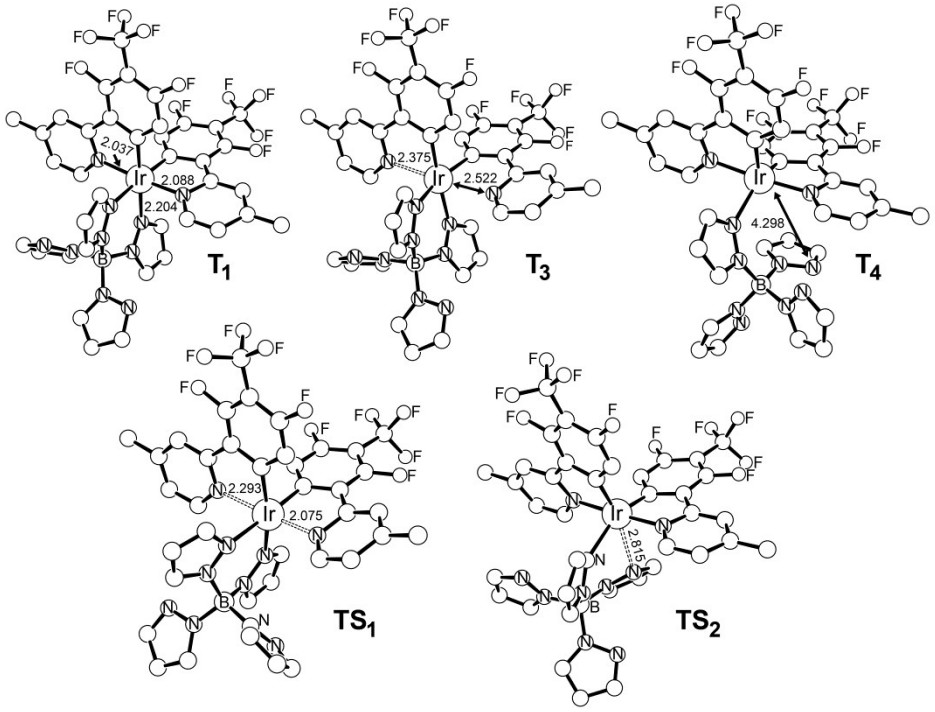

Fig. S9 Optimized structures of triplet states and transition states $\mathbf{TS_1}$ and $\mathbf{TS_2}$ for **bor**.

Table S6. Computed energy components of the optimized structures in eV.

	E(SCF) cc-pVTZ(-f)	ZPE	-TS 298.15 K	G(solv)	G(sol)
pic–S_0	-72085.063	12.163	-3.288	-0.974	-72077.162
pic–T_1	-72082.337	12.049	-3.337	-0.902	-72074.527
pic–T_2	-72082.026	12.042	-3.286	-0.876	-72074.145
pic–TS_1	-72081.892	12.008	-3.364	-0.830	-72074.078
pic–TS_2	-72082.249	12.047	-3.340	-0.859	-72074.401
pic–T_3	-72082.227	12.093	-3.426	-0.847	-72074.407
pic–T_4	-72082.264	12.077	-3.440	-0.855	-72074.481
bor–S_0	-85453.623	16.505	-3.892	-0.814	-85441.824
bor–T_1	-85450.838	16.399	-3.939	-0.783	-85439.161
bor–TS_1	-85450.490	16.360	-3.905	-0.784	-85438.819
bor–TS_2	-85450.020	16.387	-3.876	-0.941	-85438.450
bor–T_3	-85450.715	16.388	-4.079	-0.789	-85439.195
bor–T_4	-85450.032	16.393	-3.937	-0.963	-85438.538
acac–S_0	-69606.304	12.666	-3.289	-0.601	-69597.528
acac–T_1	-69603.584	12.551	-3.330	-0.558	-69594.921
acac–T_2	-69603.650	12.598	-3.391	-0.576	-69595.019
acac–TS_1	-69603.361	12.555	-3.452	-0.555	-69594.813
acac–TS_2	-69603.591	12.566	-3.369	-0.551	-69594.944
acac–T_3	-69603.493	12.598	-3.427	-0.580	-69594.902
acac–T_4	-69603.568	12.589	-3.435	-0.559	-69594.973

Table S7. Cartesian coordinates of the optimized geometries for each complex tabulating in x, y and z coordinates.

pic–S_0				**pic–T_1**			
Ir	-0.767359516	-2.414804349	0.766714037	Ir	-0.769129521	-2.427589479	0.816050564
C	-1.987805722	-2.184584787	2.351359709	C	-2.042160317	-2.201559165	2.331398576
C	-2.229043492	-0.821316230	2.714313208	C	-2.233330482	-0.782600660	2.720513973
C	-2.650822502	-3.187685898	3.074919869	C	-2.774239261	-3.187735062	2.996311484
C	-1.511489981	0.184150404	1.921284251	C	-1.523958901	0.177172794	1.981494562
C	-3.099999149	-0.535645425	3.776096816	C	-3.134932499	-0.515426782	3.814584155
C	-3.504132993	-2.850385763	4.110937428	C	-3.651251815	-2.851445191	4.013029163
H	-2.511062080	-4.238711948	2.847522975	H	-2.659617812	-4.236832224	2.745094877
C	-1.565839307	1.578564268	2.055283009	C	-1.530855226	1.608123780	2.116201770
N	-0.714804003	-0.362272474	0.954153040	N	-0.701276593	-0.391349814	0.967607293
C	-3.753079600	-1.527603727	4.510004961	C	-3.845689923	-1.504329142	4.452475172
F	-3.328664154	0.754029106	4.106403632	F	-3.285717668	0.770229258	4.202677761
F	-4.133243352	-3.835963371	4.775701246	F	-4.357751790	-3.816510882	4.636204702
C	-0.811710612	2.410922386	1.227512731	C	-0.777924071	2.414759972	1.300844135
H	-2.204732299	2.010250461	2.811591299	H	-2.151711488	2.047400411	2.884414542
C	0.026633821	0.426892634	0.155347975	C	0.035618622	0.402079620	0.184823078
C	0.004410636	1.807354900	0.260917383	C	0.035888350	1.785444530	0.302278787
H	0.632069266	-0.096808309	-0.576439321	H	0.642868025	-0.110607304	-0.554678394
H	0.613455706	2.402940217	-0.411608100	H	0.657141229	2.373802273	-0.364465639
O	0.406177453	-2.397262233	-1.056729901	O	0.378263802	-2.449544521	-1.015282140
C	-0.237632974	-2.310431421	-2.179716636	C	-0.252591802	-2.367538154	-2.147481438
C	-1.753016117	-2.153941401	-2.050187669	C	-1.762412998	-2.169792255	-2.028283514
O	0.242654488	-2.315434092	-3.308654811	O	0.239169631	-2.413343766	-3.268906128
C	-2.549683636	-1.994142265	-3.182350402	C	-2.548924672	-1.999620706	-3.165807275
N	-2.282061587	-2.156757732	-0.808764738	N	-2.297376418	-2.154294504	-0.790550170
C	-3.922666903	-1.828913130	-3.029038964	C	-3.917849697	-1.797434668	-3.018695917
H	-2.054444321	-2.002683561	-4.146727315	H	-2.051526830	-2.028456377	-4.128683215
C	-3.609406051	-1.996245354	-0.655104043	C	-3.619418369	-1.960682606	-0.642467000
C	-4.462191477	-1.829128251	-1.740706793	C	-4.462913769	-1.775930383	-1.733054728
H	-4.565135940	-1.699958367	-3.895432880	H	-4.552707207	-1.656875031	-3.888850094
H	-3.975823598	-2.005195671	0.366150251	H	-3.989104876	-1.963131464	0.378008707
H	-5.526541619	-1.701060034	-1.573075029	H	-5.524154861	-1.618449719	-1.571447621
C	0.818673081	-2.784412913	1.951589668	C	0.833637412	-2.785748019	1.972530901

C	1.196327859	-4.159401912	2.018573885	C	1.215945352	-4.159630094	2.039476242
C	1.601065018	-1.848049189	2.631968750	C	1.630299376	-1.832845993	2.610607381
C	0.328802315	-5.094146535	1.298135620	C	0.343912737	-5.107429641	1.339455446
C	2.339110660	-4.504588085	2.746453286	C	2.381571228	-4.489526320	2.736109734
C	2.725571436	-2.241893880	3.344038919	C	2.780741013	-2.213744492	3.288578112
H	1.363833250	-0.790644501	2.617488997	H	1.384399142	-0.778211494	2.581130279
C	0.482427117	-6.485510400	1.205619324	C	0.515190876	-6.496349666	1.247630223
N	-0.731418793	-4.490139700	0.680216201	N	-0.726486229	-4.514706221	0.731148791
C	3.132659031	-3.579540381	3.431668668	C	3.194925234	-3.549020056	3.376408086
F	2.733298828	-5.797190959	2.814259566	F	2.782596592	-5.778233218	2.812077277
F	3.434271450	-1.284972466	3.963496821	F	3.507365787	-1.248619506	3.869942709
C	-0.425605131	-7.266217698	0.493547460	C	-0.389228923	-7.285376229	0.537539147
H	1.325799197	-6.951459490	1.694019902	H	1.365978649	-6.953847769	1.730633787
C	-1.617346641	-5.239176640	-0.001561975	C	-1.605582016	-5.270029902	0.049304451
C	-1.506416508	-6.612976592	-0.115594103	C	-1.478073176	-6.642643753	-0.068141143
H	-2.433696873	-4.699467956	-0.465393076	H	-2.430569962	-4.737963177	-0.408568116
H	-2.251827121	-7.164549138	-0.679845815	H	-2.219142503	-7.202193027	-0.630233673
C	4.351549177	-4.062341441	4.177405255	C	4.444315457	-4.019654487	4.082362555
F	4.982471477	-3.076988621	4.839365121	F	5.116122786	-3.019490325	4.676159326
F	4.028025842	-5.009191204	5.088763525	F	4.151490413	-4.929033381	5.039610582
F	5.254110462	-4.622019662	3.339088786	F	5.296315294	-4.619002573	3.220336182
C	-4.713414596	-1.278117134	5.646410367	C	-4.826679845	-1.267865888	5.579447701
F	-4.365407176	-1.986798783	6.743151819	F	-4.473250145	-1.968421289	6.678424452
F	-4.779873559	0.013652554	6.014835276	F	-4.931288172	0.020131885	5.945179163
F	-5.969008590	-1.661720373	5.314019704	F	-6.063891802	-1.682934263	5.223283718
C	-0.856409635	3.909325232	1.383328581	C	-0.782672310	3.914705589	1.426365249
H	0.015612578	4.263896450	1.946308614	H	0.224504858	4.297102748	1.634656528
H	-0.839096491	4.409858013	0.410251277	H	-1.113677070	4.387901771	0.493064934
H	-1.751797936	4.229564102	1.922052158	H	-1.444762215	4.249227183	2.229209192
C	-0.248129899	-8.756601431	0.361736691	C	-0.199818657	-8.774057504	0.403910635
H	0.499230871	-9.136620833	1.062002532	H	0.556195007	-9.148287143	1.097827504
H	-1.190650864	-9.284439973	0.540713965	H	-1.136605276	-9.309382830	0.590298794
H	0.079455007	-9.015083418	-0.652514362	H	0.121189246	-9.028948318	-0.613269001

pic–T_2

Ir	-0.731212671	-2.286012399	0.525186829

pic–TS_1

Ir	-0.582936134	-2.343619954	1.135622356

C	-2.001548605	-1.725252764	2.019762077	C	-1.802271950	-2.515762837	2.764993365
C	-2.095541331	-0.327311351	2.252601086	C	-2.359788663	-1.270703314	3.200771211
C	-2.785193306	-2.588132504	2.794931389	C	-2.093753605	-3.684339787	3.480699924
C	-1.261032509	0.512942400	1.389684766	C	-2.055828287	-0.082914050	2.399898207
C	-2.944409066	0.143814540	3.265573307	C	-3.149608927	-1.263528922	4.362409823
C	-3.614232156	-2.071907641	3.778588615	C	-2.926684843	-3.628367672	4.584891188
H	-2.768555233	-3.663027966	2.655485979	H	-1.689813326	-4.644997667	3.180415991
C	-1.224342043	1.912248943	1.352498411	C	-2.845988402	1.069376647	2.312619318
N	-0.465966290	-0.205170365	0.544572792	N	-0.923886771	-0.223963064	1.617512485
C	-3.708781889	-0.703325198	4.069175649	C	-3.468251404	-2.424939888	5.068845276
F	-3.030623967	1.472809833	3.479182628	F	-3.611328521	-0.079659589	4.818801837
F	-4.364642282	-2.926486657	4.491895073	F	-3.244218000	-4.770005737	5.226285187
C	-0.378812566	2.584577949	0.470743181	C	-2.529277821	2.099553951	1.428004670
H	-1.869578725	2.472427471	2.012689876	H	-3.724298708	1.151063193	2.941380996
C	0.371074926	0.429825796	-0.299155850	C	-0.627889903	0.770961816	0.735118475
C	0.441540735	1.811068244	-0.360920380	C	-1.377233694	1.920830599	0.623490075
H	0.978300443	-0.212495600	-0.925205601	H	0.264112675	0.611887985	0.136231472
H	1.124964231	2.275210984	-1.064451164	H	-1.059653154	2.695717265	-0.068822539
O	0.542083405	-2.358102921	-1.057847745	O	0.369543573	-2.182837503	-0.733854049
C	-0.052891938	-2.358564760	-2.307651984	C	-0.333588054	-1.934313624	-1.806641739
C	-1.456235390	-2.126009931	-2.340128077	C	-1.835257358	-1.917810246	-1.572885974
O	0.704997718	-2.575075143	-3.278249484	O	0.104674584	-1.733031146	-2.929363544
C	-2.194470089	-2.009657847	-3.550854978	C	-2.724666669	-1.716588768	-2.624228734
N	-2.112468936	-1.997858165	-1.113558940	N	-2.256899289	-2.099908823	-0.305214744
C	-3.536797600	-1.738455641	-3.514016955	C	-4.091186791	-1.705130926	-2.357101594
H	-1.654588020	-2.134499064	-4.483752256	H	-2.311449372	-1.574157898	-3.616391386
C	-3.432862475	-1.713045032	-1.101429655	C	-3.574965021	-2.082789765	-0.041277948
C	-4.185016659	-1.575423901	-2.248730380	C	-4.522269937	-1.891143133	-1.042760549
H	-4.105795515	-1.642708881	-4.434121922	H	-4.809879982	-1.552342547	-3.156993065
H	-3.881247224	-1.609772424	-0.116957266	H	-3.857397923	-2.226923058	0.995566590
H	-5.243255518	-1.350688565	-2.178448514	H	-5.576978580	-1.887618962	-0.788210239
C	0.724182267	-2.754285232	1.872832014	C	1.106026784	-2.592304976	2.203098921
C	0.884145777	-4.156328997	2.079977341	C	1.743749944	-3.865941222	2.098754209
C	1.574627297	-1.879384337	2.544885382	C	1.711372981	-1.584190209	2.957439640
C	-0.037110748	-5.023083501	1.337675504	C	1.075854679	-4.882433216	1.271448593
C	1.894063114	-4.594749986	2.942305449	C	2.954748096	-4.044268698	2.770767233

C	2.563842755	-2.363078561	3.393420722	C	2.924502812	-1.811665862	3.594748442
H	1.498954274	-0.804962646	2.420775138	H	1.248035434	-0.608290774	3.049618130
C	-0.049812449	-6.421224828	1.308850126	C	1.610280571	-6.117516103	0.873977285
N	-0.960540729	-4.331974923	0.592151536	N	-0.169861320	-4.519654689	0.862506050
C	2.752959988	-3.730527096	3.628823340	C	3.583698802	-3.045275757	3.523773088
F	2.079623587	-5.917920244	3.147133223	F	3.585237711	-5.239503574	2.721109459
F	3.353857694	-1.464842984	3.998761829	F	3.464587685	-0.802203372	4.292240061
C	-0.978534766	-7.120259201	0.531476685	C	0.881874720	-6.977300550	0.050815187
H	0.682641087	-6.962540930	1.890521912	H	2.601235462	-6.398198193	1.200379005
C	-1.867317634	-4.993939567	-0.151522614	C	-0.880135898	-5.342327626	0.074926174
C	-1.910273462	-6.375511921	-0.202400200	C	-0.401685015	-6.570994263	-0.347976713
H	-2.551918598	-4.372698950	-0.715524107	H	-1.865624246	-4.988107658	-0.212762488
H	-2.658022810	-6.862281611	-0.819553251	H	-1.017982973	-7.202908349	-0.980356505
C	-0.340178603	4.090376199	0.431158749	C	4.902735620	-3.358297347	4.192136364
H	0.525594494	4.468707641	0.988054600	F	5.412474025	-2.310312218	4.858576178
H	-0.252312954	4.457479718	-0.595827683	F	4.772387795	-4.372090513	5.076798695
H	-1.238180207	4.524266637	0.878103825	F	5.827302218	-3.744252845	3.284601076
C	-0.947159059	-8.624894164	0.462832840	C	-4.341743589	-2.474870355	6.301540642
H	-0.757585135	-9.071892457	1.503789551	F	-3.679437600	-3.019562343	7.344777485
H	-1.927542444	-9.023427514	0.043824252	F	-4.782539733	-1.268198206	6.694874482
H	-0.085988540	-8.955708077	-0.226339672	F	-5.432323872	-3.244483833	6.080317911
C	-4.642249224	-0.237052978	5.161985952	C	-3.375849462	3.340318455	1.314130148
F	-4.485970843	-0.975207870	6.281724562	H	-2.783292595	4.245105648	1.498811287
F	-4.448716472	1.048749120	5.506630119	H	-3.808095010	3.443747654	0.310402586
F	-5.935154018	-0.360111532	4.784780369	H	-4.200152370	3.328288110	2.032862909
C	3.817143061	-4.306777290	4.531532570	C	1.456925852	-8.288588502	-0.419127359
F	4.489453770	-3.363039776	5.211614785	H	2.356673245	-8.557013147	0.139525562
F	3.280895270	-5.150087872	5.442547024	H	0.729108651	-9.099968184	-0.313650921
F	4.726148938	-5.017967768	3.826992270	H	1.725556041	-8.232143401	-1.481015885

pic–TS_2

Ir	-0.723070446	-2.400750156	0.906485054
C	-2.229633014	-2.197300415	2.206048165
C	-2.386855235	-0.840407619	2.692059887
C	-2.987454287	-3.230206160	2.804462505
C	-1.607404888	0.175192838	2.020148750

pic–T_3

Ir	-0.790076484	-2.550876862	1.044759197
C	-1.953262525	-1.716183292	2.507145509
C	-2.185949780	-0.317884630	2.612449606
C	-2.561944495	-2.571732397	3.439578051
C	-1.555699301	0.562501900	1.603915606

C	-3.267303287	-0.620703622	3.768386815	C	-2.982169765	0.151176192	3.671748129
C	-3.862152378	-2.939980425	3.823898070	C	-3.348973082	-2.054677298	4.454758173
H	-2.905689179	-4.259019266	2.470807551	H	-2.421839536	-3.647847850	3.408056395
C	-1.666123898	1.572618813	2.188816231	C	-1.814035870	1.931749534	1.421217260
N	-0.736927323	-0.351289316	1.085064081	N	-0.675097381	-0.071982214	0.803385875
C	-4.034025539	-1.629779267	4.342748911	C	-3.582784905	-0.684320285	4.616112374
F	-3.380101729	0.631139988	4.261959291	F	-3.178259555	1.479671914	3.804495401
F	-4.621128055	-3.922462566	4.350745778	F	-3.915577193	-2.903989678	5.327777036
C	-0.883782306	2.424554988	1.422003115	C	-1.140816779	2.654917005	0.436426994
H	-2.345979054	1.981931556	2.922595914	H	-2.546988033	2.430186766	2.038663611
C	0.031249644	0.471703994	0.337667439	C	-0.010125274	0.609982631	-0.135385354
C	-0.012871816	1.843494950	0.470693669	C	-0.203221299	1.970390414	-0.346865301
H	0.683791368	-0.023723727	-0.373052523	H	0.676188964	0.024276852	-0.737524759
H	0.623812813	2.459996265	-0.155759858	H	0.360057589	2.480746994	-1.122585156
O	0.274882257	-2.333707766	-1.018769615	O	0.144578577	-2.161121744	-0.948751764
C	-0.315601118	-2.170738563	-2.166352302	C	-0.651243102	-2.143264432	-1.973885758
C	-1.819267664	-1.967033663	-2.086325942	C	-2.127797980	-2.342974601	-1.658743340
O	0.233447558	-2.149920589	-3.261289309	O	-0.321771117	-1.979353625	-3.144686722
C	-2.559766095	-1.683229815	-3.234398055	C	-3.076072286	-2.311398652	-2.679229617
N	-2.386036814	-2.059294463	-0.875286025	N	-2.474783837	-2.551393648	-0.371461811
C	-3.931586040	-1.482565852	-3.111072114	C	-4.417834109	-2.501979478	-2.365422311
H	-2.034289322	-1.627950521	-4.181017652	H	-2.719280654	-2.137493559	-3.687928949
C	-3.706452386	-1.864308260	-0.751880715	C	-3.771968940	-2.735458805	-0.065046993
C	-4.517194398	-1.574273062	-1.846329924	C	-4.770646203	-2.719881741	-1.032424022
H	-4.537481243	-1.256140008	-3.983945032	H	-5.177023194	-2.481775525	-3.141975424
H	-4.106526573	-1.947683060	0.254530487	H	-3.997346439	-2.891131143	0.984309343
H	-5.582720652	-1.423358085	-1.705998735	H	-5.803794315	-2.873811473	-0.738910331
C	0.987877807	-2.794157871	1.886132392	C	0.858994358	-2.674213627	2.225924539
C	1.293890820	-4.187538623	2.002103105	C	1.687327949	-3.829316852	2.056727058
C	1.843895647	-1.854124427	2.471578905	C	1.247223801	-1.718434847	3.168129070
C	0.378421843	-5.107510567	1.326057741	C	1.265187578	-4.823003437	1.053365742
C	2.440172272	-4.548752709	2.712889923	C	2.835801894	-3.941607667	2.848867056
C	2.982634798	-2.268294287	3.147184407	C	2.393462339	-1.880888892	3.934090975
H	1.654404406	-0.789492133	2.397384068	H	0.659491097	-0.822924719	3.331054804
C	0.514728169	-6.497200911	1.203938002	C	1.954161997	-5.990568934	0.683199890
N	-0.689369319	-4.476885269	0.747874123	N	0.088658838	-4.527041160	0.444820742

C	3.314859918	-3.624003133	3.295048894	C	3.222090089	-3.001313498	3.810366416
F	2.760415870	-5.853189865	2.861814064	F	3.652442314	-5.012454242	2.713792574
F	3.785288291	-1.322710296	3.657650901	F	2.693895391	-0.917477995	4.819074878
C	-0.411419220	-7.249590816	0.483343999	C	1.445917187	-6.842984822	-0.297878284
H	1.361406821	-6.983644038	1.666767847	H	2.896699742	-6.224085754	1.154974181
C	-1.587631071	-5.195693557	0.049706983	C	-0.416706652	-5.344291332	-0.488161207
C	-1.488232987	-6.566370982	-0.103946024	C	0.217803038	-6.508608444	-0.886793760
H	-2.402917174	-4.631124823	-0.385858727	H	-1.357069550	-5.035106836	-0.932835839
H	-2.243355989	-7.095568073	-0.676500026	H	-0.228097707	-7.135454640	-1.653197991
C	4.538862748	-4.134005164	4.020162505	C	4.480881114	-3.235127155	4.609151446
F	5.285171702	-3.147423318	4.542120505	F	4.657814174	-2.327466349	5.580914622
F	4.194870308	-4.957826899	5.035320816	F	4.469259191	-4.449520291	5.200805614
F	5.334947195	-4.843654941	3.189563862	F	5.578276476	-3.195819566	3.822262798
C	-5.031884473	-1.429384319	5.456145394	C	-4.440207859	-0.226327878	5.771633347
F	-4.721146459	-2.184537361	6.533128018	F	-3.931547585	-0.649980001	6.948101215
F	-5.121381129	-0.155852501	5.876842982	F	-4.568711770	1.108652185	5.852513639
F	-6.271454774	-1.804112062	5.058994661	F	-5.686669742	-0.739336066	5.676987679
C	-0.954278987	3.920972695	1.582973429	C	-1.413999509	4.124393169	0.229944365
H	0.023968130	4.334232031	1.856601465	H	-0.529953053	4.723525781	0.478837369
H	-1.252781102	4.403925989	0.644515776	H	-1.663454460	4.335309330	-0.816264019
H	-1.671779674	4.209196854	2.355386174	H	-2.241976986	4.470713400	0.855129591
C	-0.258298007	-8.738797819	0.315614323	C	2.203330793	-8.071403149	-0.734612121
H	0.519933084	-9.140315021	0.968629713	H	3.011861459	-8.313248929	-0.040852806
H	-1.196646854	-9.258690308	0.536478001	H	1.540360114	-8.939860143	-0.811879073
H	0.009902251	-8.983963846	-0.719157906	H	2.646926530	-7.913619647	-1.726256861

pic–T_4

Ir	-0.639677116	-2.404470098	1.124694836
C	-2.267568046	-2.160293068	2.293517247
C	-2.479522819	-0.804082243	2.713879240
C	-3.075222260	-3.171265715	2.852794203
C	-1.627931633	0.198172850	2.076870202
C	-3.459172017	-0.538736604	3.681414543
C	-4.039187876	-2.847768980	3.785353651
H	-2.964932001	-4.212107474	2.568612888
C	-1.725534609	1.593648211	2.179609504

bor–S_0

C	1.570786253	0.231242455	1.928750643
C	2.437683513	-0.794708714	2.317395071
C	3.223912869	-0.668074640	3.456143558
C	3.198357946	0.473684170	4.267135693
C	2.336146577	1.496299196	3.855748088
C	1.516426489	1.413306206	2.726435092
C	0.565707579	2.439398781	2.280075309
C	0.284262114	3.655769014	2.912664600
C	-0.681266854	4.525962709	2.399388833

N	-0.665860879	-0.353439083	1.272643523	C	-1.345217977	4.142263130	1.229463381
C	-4.265414540	-1.533292131	4.239622908	C	-1.029886576	2.932439088	0.631830252
F	-3.638953262	0.733783436	4.095509782	N	-0.099440721	2.102953029	1.131686552
F	-4.821339121	-3.824247021	4.282476645	F	2.323523933	2.612124832	4.620390060
C	-0.869257984	2.428061133	1.465280998	F	4.031359160	-1.693430790	3.769780482
H	-2.488040627	2.020754066	2.814901746	Ir	0.364640973	0.257027143	0.305081559
C	0.166884099	0.443954484	0.570394949	C	1.975005732	0.880610268	-0.753116278
C	0.095990490	1.823157097	0.641670231	C	2.448068918	2.188510280	-0.888596617
H	0.877367640	-0.074410877	-0.063309390	C	3.577764938	2.465616176	-1.649025491
H	0.786148612	2.421847282	0.055753286	C	4.302496725	1.467084075	-2.310573783
O	0.153804072	-2.251023484	-0.881704353	C	3.824853258	0.160939810	-2.154195960
C	-0.427678251	-2.131271059	-2.040028357	C	2.688772427	-0.168261785	-1.410050937
C	-1.940866818	-1.979297865	-2.037321505	C	2.125717724	-1.516974774	-1.263532034
O	0.163690110	-2.106153044	-3.114308707	C	2.599321914	-2.694876344	-1.854882263
C	-2.597181429	-1.682565566	-3.235580576	C	1.934572714	-3.909045773	-1.676010631
N	-2.594535575	-2.123131806	-0.879362321	C	0.775301463	-3.905517366	-0.891552642
C	-3.978865129	-1.520272621	-3.216935103	C	0.343987771	-2.720179794	-0.319400157
H	-2.004825310	-1.589639514	-4.138629421	N	1.001291772	-1.558450961	-0.485320512
C	-3.924201058	-1.968723712	-0.862279350	F	4.526836858	-0.808913872	-2.783298786
C	-4.659844393	-1.665471787	-2.006533980	F	3.967095625	3.746855610	-1.738657865
H	-4.519457281	-1.283514643	-4.129237944	B	-3.175998178	-0.440873043	-0.388221188
H	-4.407643740	-2.095116410	0.104065177	N	-2.151599762	-0.351197294	-1.558192406
H	-5.737014828	-1.543650636	-1.945960255	N	-3.775307057	0.964903630	-0.181778374
C	1.218674315	-2.831101467	1.922972256	N	-2.546670800	-0.954927256	0.932407073
C	1.503970750	-4.226735646	1.979523611	N	-4.280147472	-1.422157117	-0.793968801
C	2.123865452	-1.926557350	2.480782612	C	-3.239025634	-1.622265164	1.884889274
C	0.513106643	-5.119243274	1.362142561	C	-2.451679638	-1.734389771	3.015276292
C	2.688829864	-4.630799890	2.597238184	C	-1.260326220	-1.085428452	2.676714781
C	3.296766150	-2.378621678	3.073521252	N	-1.320524475	-0.610573587	1.424686009
H	1.949155557	-0.856063232	2.455745427	N	-3.964423565	-2.719234404	-1.084451734
C	0.639944111	-6.500085951	1.163085791	C	-5.124132819	-3.305313239	-1.372168412
N	-0.611861024	-4.473639064	0.932640599	C	-6.208128869	-2.404687928	-1.272003789
C	3.615357033	-3.740167657	3.154310066	C	-5.624459753	-1.210990354	-0.898369307
F	2.997305540	-5.944782732	2.684244134	N	-0.960662897	0.312779908	-1.474518162
F	4.139927082	-1.462095836	3.572326940	C	-0.530870629	0.494181041	-2.731674817
C	-0.359529732	-7.228887837	0.517607254	C	-1.442707158	-0.041885761	-3.647387880

H	1.535430686	-6.999064974	1.504699526
C	-1.579570154	-5.167133907	0.305830960
C	-1.495163014	-6.530928055	0.085263226
H	-2.431837936	-4.583549290	-0.020191618
H	-2.307045479	-7.040139309	-0.424552657
C	4.867957087	-4.295264143	3.790588463
F	5.667502126	-3.339212367	4.291062868
F	4.566624473	-5.137723722	4.804489766
F	5.596667786	-5.000574892	2.896692117
C	-5.355161843	-1.300701965	5.257507875
F	-5.162353169	-2.059176489	6.359614786
F	-5.443222819	-0.022969867	5.665468410
F	-6.564927381	-1.641787112	4.753406759
C	-0.976321985	3.928618014	1.559974251
H	-0.041133337	4.365297693	1.928834191
H	-1.170360498	4.369872452	0.575541565
H	-1.781547555	4.232505109	2.233291270
C	-0.216795052	-8.707651616	0.266708555
H	0.617336687	-9.133185037	0.829273787
H	-1.130237848	-9.244676017	0.542833988
H	-0.038310185	-8.900403499	-0.798002631

C	-2.452800356	-0.568844732	-2.861365846
C	-3.987808572	1.932896794	-1.120699090
C	-4.730310026	2.937508768	-0.530643923
C	-4.934719714	2.482110399	0.791074441
N	-4.365512657	1.296800328	0.998156628
H	2.524091470	-1.711740273	1.745675613
H	0.816188615	3.912817872	3.816927708
H	-2.115787631	4.763683036	0.785550263
H	-1.531306414	2.594840921	-0.265681013
H	1.951332563	3.023213902	-0.406609271
H	3.487250563	-2.653298006	-2.468617145
H	0.199808359	-4.811489495	-0.731703811
H	-0.555300565	-2.675740453	0.281081803
H	-4.244209400	-1.960123210	1.690374199
H	-2.704911007	-2.211758254	3.949376394
H	-0.361068805	-0.953091117	3.258323022
H	-5.142386824	-4.354338871	-1.641688142
H	-7.257268484	-2.596536595	-1.443381234
H	-6.056585281	-0.243945528	-0.688710855
H	0.417027575	0.978981086	-2.909687118
H	-1.372725312	-0.053868220	-4.724427257
H	-3.363660526	-1.079670455	-3.130866874
H	-3.608822999	1.833810789	-2.127867479
H	-5.074490247	3.854459691	-0.987210306
H	-5.469656740	2.967967530	1.597770012
C	4.043906688	0.672885971	5.501182411
F	4.753238021	-0.420404935	5.829016482
F	4.924628378	1.686410270	5.337251407
F	3.281546440	0.988032957	6.573512216
C	5.529177041	1.704248815	-3.156535105
F	5.852409891	3.004612784	-3.254537338
F	6.607451983	1.060002820	-2.655425339
F	5.349608257	1.242910594	-4.416875416
C	-1.017966949	5.815027964	3.104852956
H	-0.132410153	6.263569377	3.564405875
H	-1.458819515	6.542495474	2.417745196

H	-1.746003603	5.633835109	3.905354781
C	2.454773040	-5.180095430	-2.296090498
H	3.116118065	-5.704932469	-1.595877965
H	1.637777195	-5.862484925	-2.547845228
H	3.030849333	-4.977134612	-3.202856063

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C	1.614235436	0.524586934	1.968260407
C	2.587672103	-0.423691843	2.291901044
C	3.344406323	-0.294232149	3.450289192
C	3.177479479	0.770134085	4.345836330
C	2.206263751	1.715267719	3.998698481
C	1.412066058	1.627329353	2.851186320
C	0.355491244	2.573614099	2.467927073
C	-0.071144192	3.696067087	3.186862748
C	-1.117042483	4.495428242	2.719847512
C	-1.713088015	4.139805469	1.505497643
C	-1.257620699	3.022116567	0.825134781
N	-0.252613800	2.259036208	1.284288455
F	2.053965122	2.757628044	4.846367030
F	4.262304211	-1.240418998	3.699064739
Ir	0.420380692	0.525829376	0.334902575
C	1.945259451	1.382225434	-0.669697970
C	2.293533268	2.721306435	-0.720318708
C	3.401292723	3.161363271	-1.450832340
C	4.235630314	2.270083002	-2.169793089
C	3.909504699	0.929760123	-2.118755802
C	2.784680235	0.408425571	-1.387789249
C	2.410930966	-0.934202775	-1.295460763
C	3.043564983	-2.080747467	-1.901387477
C	2.479372739	-3.321954139	-1.856680783
C	1.214809484	-3.454466410	-1.172498181
C	0.641622016	-2.357067746	-0.541131222
N	1.199768108	-1.143993031	-0.533758514
F	4.693527582	0.071912617	-2.808943657
F	3.659912827	4.478574102	-1.464208197

bor–TS_1

C	1.991884915	0.038993396	1.659202100
C	2.613237835	-1.117935500	2.128867375
C	3.579734848	-1.039887298	3.127517838
C	3.960977184	0.177779037	3.708794911
C	3.315298454	1.321963517	3.230983702
C	2.345015032	1.298655587	2.222712990
C	1.666597430	2.451584549	1.652317952
C	2.091541623	3.780428714	1.684457774
C	1.388335122	4.787867545	1.021466583
C	0.214418437	4.402344947	0.315307737
C	-0.189621164	3.094800646	0.297757667
N	0.511339071	2.094950226	0.935185812
F	3.653581023	2.501300884	3.798728118
F	4.157606831	-2.187658207	3.523831539
Ir	0.569948925	0.157165165	0.195721948
C	2.146301695	0.179767069	-1.108192764
C	2.842240434	1.351023340	-1.414736513
C	3.896053605	1.328513107	-2.321101738
C	4.316738349	0.148988530	-2.943220480
C	3.613259917	-1.012193251	-2.604056431
C	2.533039504	-1.045597047	-1.714334490
C	1.746879403	-2.248540158	-1.373816487
C	1.960344324	-3.542520210	-1.872260175
C	1.115899762	-4.594280458	-1.513821613
C	0.049038146	-4.308445615	-0.652611801
C	-0.110096745	-3.015226524	-0.179157488
N	0.721319394	-2.017805411	-0.514242614
F	4.031954361	-2.150209326	-3.201562371
F	4.513742395	2.489023936	-2.585627503

B	-3.051145199	-0.427010893	-0.416037395	B	-3.047071017	-0.206806711	0.001515367
N	-2.050617782	-0.136903249	-1.576652611	N	-2.188527052	-0.316767755	-1.292229983
N	-3.789994962	0.883716856	-0.078038491	N	-3.457786846	1.262110358	0.181136577
N	-2.363046353	-0.996239267	0.852397862	N	-2.302673263	-0.705807979	1.277449425
N	-4.058312443	-1.469452982	-0.910445873	N	-4.286510584	-1.088258035	-0.167654606
C	-2.980554181	-1.812548752	1.738158408	C	-2.935022725	-1.168829787	2.374949704
C	-2.181694674	-1.945046264	2.857546172	C	-2.019761582	-1.282422862	3.412326719
C	-1.063533303	-1.151269009	2.584603638	C	-0.816052484	-0.845193803	2.867020169
N	-1.177255635	-0.574986457	1.380035803	N	-0.988398928	-0.486766434	1.581436859
N	-3.621040123	-2.697523711	-1.318954550	N	-4.142189625	-2.436500373	-0.338563925
C	-4.720624818	-3.364381799	-1.661253935	C	-5.381773840	-2.909338140	-0.445555308
C	-5.885891393	-2.586243153	-1.479736107	C	-6.347127655	-1.882658314	-0.344291109
C	-5.417778397	-1.381093210	-0.996493632	C	-5.603956535	-0.733373046	-0.165444546
N	-0.911375498	0.607090225	-1.441956507	N	-0.946858500	0.234234673	-1.425586783
C	-0.504816588	0.923209533	-2.679730006	C	-0.669696080	0.256519780	-2.736042701
C	-1.381841219	0.399749576	-3.634122006	C	-1.736508288	-0.270265945	-3.472887735
C	-2.343366676	-0.266477433	-2.893041693	C	-2.675830053	-0.622809358	-2.519278532
C	-4.152442263	1.886527722	-0.930485714	C	-3.634653524	2.215653983	-0.780790661
C	-4.978548345	2.751276910	-0.239110575	C	-4.193064008	3.324252387	-0.176429274
C	-5.070416141	2.180671022	1.049965632	C	-4.331359785	2.946037601	1.177634120
N	-4.363606119	1.056880003	1.144113925	N	-3.896777696	1.706601307	1.390858472
H	2.781966164	-1.277591131	1.652956083	H	2.378754128	-2.096499155	1.724580691
H	0.414131649	3.936805678	4.121524504	H	2.991202842	4.021921981	2.237298497
H	-2.536592217	4.710669787	1.090642385	H	-0.396448981	5.148071796	-0.185842101
H	-1.703665865	2.704805489	-0.107952177	H	-1.103412074	2.782081817	-0.192804223
H	1.712134068	3.473783886	-0.197523517	H	2.589732831	2.302068106	-0.958676883
H	3.983335941	-1.929344903	-2.413001026	H	2.784651574	-3.724517689	-2.545940499
H	0.695972656	-4.406334813	-1.139016662	H	-0.656568342	-5.077356707	-0.353522022
H	-0.303950816	-2.456640836	-0.021332719	H	-0.932579332	-2.757694919	0.477434113
H	-3.946397707	-2.233108003	1.508790548	H	-3.993897910	-1.370927708	2.348692379
H	-2.380123601	-2.529281005	3.742780247	H	-2.207102295	-1.624554786	4.418438014
H	-0.177469656	-0.985590989	3.177739100	H	0.163609662	-0.779383178	3.313656134
H	-4.639305165	-4.380777071	-2.026636192	H	-5.540447861	-3.971120312	-0.589743104
H	-6.912787672	-2.862255482	-1.669433478	H	-7.423009803	-1.967413475	-0.389105817
H	-5.940281902	-0.483988417	-0.699388607	H	-5.905078320	0.294018754	-0.024783066
H	0.402625305	1.492227886	-2.815418685	H	0.285931540	0.626377559	-3.077004022

H	-1.320332413	0.484326679	-4.708295668	H	-1.810709859	-0.385835129	-4.543441478
H	-3.213491076	-0.822559403	-3.204532729	H	-3.655720295	-1.061671623	-2.622055877
H	-3.811191495	1.903838468	-1.955833281	H	-3.360373943	2.035254428	-1.810360116
H	-5.444654457	3.652446833	-0.611051382	H	-4.455367263	4.263492689	-0.641482426
H	-5.619913985	2.541594220	1.910572931	H	-4.723656210	3.526165570	2.003491126
C	3.985339408	0.967895056	5.605837087	C	4.993248010	0.323184948	4.800221900
F	4.800938667	-0.066789677	5.868617459	F	5.555498413	-0.846948728	5.148979519
F	4.756449463	2.076147388	5.525692508	F	5.995186736	1.149128738	4.421277768
F	3.182896819	1.126100385	6.682962252	F	4.451915070	0.854585373	5.920436537
C	5.434713132	2.697187485	-2.987821015	C	5.457275359	0.052623320	-3.929359088
F	5.645506088	4.023646844	-2.956500202	F	6.017549299	1.243956707	-4.194757236
F	6.564085855	2.101674684	-2.545502831	F	6.435296720	-0.758776125	-3.470150435
F	5.284883787	2.347259418	-4.285708318	F	5.039258040	-0.463521620	-5.107690605
C	-1.604568670	5.677158057	3.518646049	C	1.849469761	6.219161928	1.023472754
H	-0.779201101	6.186650462	4.024406229	H	2.224646875	6.520063962	0.035857038
H	-2.123605555	6.401243876	2.884845607	H	1.026037702	6.900981893	1.268885127
H	-2.309991405	5.349829895	4.292486700	H	2.653080300	6.381557492	1.746737201
C	3.122727632	-4.531667738	-2.477176491	C	1.335837025	-5.989864640	-2.039193596
H	3.407460438	-5.264504106	-1.710673016	H	1.533946207	-6.686933549	-1.216890929
H	2.429229413	-5.040397982	-3.158382323	H	0.444285073	-6.354293172	-2.561626789
H	4.020621205	-4.265107631	-3.040490217	H	2.179902268	-6.032218367	-2.731599848

bor–TS_2

C	1.643062886	-0.703584401	2.158690512
C	2.326724719	-1.863585978	2.540734039
C	3.001887038	-1.917491492	3.753934708
C	3.042752717	-0.826264534	4.631220641
C	2.362097212	0.330192662	4.225022845
C	1.661110999	0.432029934	3.022569893
C	0.948381517	1.625165518	2.543481820
C	0.720656399	2.803758088	3.260255482
C	0.015101576	3.864782178	2.689586563
C	-0.453039707	3.702485238	1.381543682
C	-0.209200668	2.515444726	0.710622093
N	0.478610082	1.503788526	1.266927602
F	2.414166863	1.380152516	5.073365135

bor–T_3

C	2.099729144	0.395401666	1.562460720
C	2.862449072	-0.757004494	1.782096273
C	3.828417050	-0.804221295	2.778538131
C	4.090810428	0.288584334	3.610059697
C	3.322647891	1.434050524	3.374855325
C	2.339640911	1.538158193	2.382611751
C	1.523803864	2.751491986	2.145317683
C	1.697521660	3.999718332	2.766090664
C	0.851499618	5.068165184	2.459499967
C	-0.175254820	4.851581784	1.530738389
C	-0.294622669	3.601997775	0.941972560
N	0.534588923	2.592072597	1.232219289
F	3.572607072	2.481708405	4.194976239

F	3.616674278	-3.064561065	4.078503818	F	4.515383338	-1.947707764	2.929314723
Ir	0.813665902	-0.310005244	0.308766829	Ir	0.646441967	0.496653026	0.120768554
C	2.117962438	0.368622593	-1.064189032	C	2.190511490	0.625680239	-1.222438977
C	2.595564034	1.684578234	-1.200151832	C	2.751908960	1.880031129	-1.493704069
C	3.661718798	1.965995274	-2.036683580	C	3.737236598	2.024230981	-2.463651653
C	4.325189821	0.970073038	-2.774194536	C	4.218036609	0.935288125	-3.196731062
C	3.843069991	-0.335493604	-2.627733980	C	3.663119063	-0.311352939	-2.882505794
C	2.758310615	-0.675079553	-1.815911899	C	2.669358102	-0.517220647	-1.919288453
C	2.209331825	-2.018361806	-1.643772611	C	2.074315445	-1.844321419	-1.613262470
C	2.561694239	-3.168725198	-2.362181991	C	2.617336645	-3.086407347	-1.982145508
C	1.928390845	-4.386433342	-2.124401170	C	1.969377785	-4.272673797	-1.630174223
C	0.927539468	-4.413036169	-1.141503664	C	0.765101927	-4.176155700	-0.920730942
C	0.612314531	-3.255741486	-0.453519580	C	0.289576540	-2.918987976	-0.573058943
N	1.237367734	-2.083986011	-0.680690143	N	0.931634427	-1.792927532	-0.897234246
F	4.489657502	-1.293137106	-3.329312764	F	4.128461351	-1.359023938	-3.600475560
F	4.054035338	3.245372568	-2.141561757	F	4.222954840	3.256440117	-2.683254653
B	-3.085894369	0.281884364	-0.517314559	B	-2.907746711	0.002778653	-0.070742611
N	-2.020986032	0.717991223	-1.547694977	N	-2.091343472	-0.021591083	-1.388860315
N	-3.527706635	1.464961378	0.387889550	N	-3.283031698	1.463790013	0.229326594
N	-2.545949348	-0.867767281	0.391578762	N	-2.122503470	-0.596422243	1.135891594
N	-4.327826875	-0.230474948	-1.273170289	N	-4.171077044	-0.838559405	-0.257290003
C	-3.385356547	-1.730842140	1.010198137	C	-2.701422695	-1.220032888	2.179358705
C	-2.701272186	-2.395859936	2.010324266	C	-1.757803576	-1.402395481	3.182414485
C	-1.409555039	-1.867400325	1.949399209	C	-0.594140470	-0.837160819	2.674171974
N	-1.314818788	-0.949596073	0.974140599	N	-0.814567631	-0.337927440	1.440840792
N	-4.155381675	-1.027577705	-2.364768728	N	-4.066060786	-2.169023342	-0.551875836
C	-5.375134434	-1.422009994	-2.714152885	C	-5.319618186	-2.608714702	-0.634327084
C	-6.364625003	-0.897616389	-1.852303285	C	-6.255530765	-1.577174079	-0.396476804
C	-5.652442200	-0.144404597	-0.941360778	C	-5.478789827	-0.461691942	-0.157295185
N	-0.957377120	-0.069193330	-1.866103514	N	-0.853961465	0.538663911	-1.505992110
C	-0.436688050	0.452707569	-2.981898414	C	-0.589382514	0.623685001	-2.815822274
C	-1.152136425	1.585751280	-3.401251702	C	-1.661274952	0.127205983	-3.567086310
C	-2.159598604	1.713016328	-2.463692464	C	-2.590265805	-0.274489866	-2.623612352
C	-4.258951591	2.564548526	0.043123325	C	-3.497087932	2.475140872	-0.661816575
C	-4.425083515	3.340976915	1.173649588	C	-4.022786915	3.545898135	0.035374327
C	-3.752429679	2.619636109	2.182613827	C	-4.102516410	3.083330347	1.368074838

N	-3.213546129	1.497067035	1.712294814	N	-3.664084221	1.831669429	1.483046215
H	2.340669599	-2.749607834	1.913776779	H	2.718017928	-1.647349553	1.180897547
H	1.091402547	2.884043068	4.272124862	H	2.492483280	4.138999665	3.483491388
H	-1.030821311	4.477848293	0.890000752	H	-0.874835893	5.639353404	1.269852223
H	-0.575147859	2.344528298	-0.294277948	H	-1.079145833	3.386092233	0.222798695
H	2.139545231	2.513144190	-0.671239682	H	2.433566651	2.771880806	-0.964249244
H	3.332593738	-3.100587259	-3.115890556	H	3.547485691	-3.128905066	-2.530365464
H	0.389290085	-5.327717769	-0.913961738	H	0.209126583	-5.063602029	-0.634012675
H	-0.162196457	-3.240175591	0.302663681	H	-0.639814248	-2.798784845	-0.022279287
H	-4.417947601	-1.798995045	0.705175597	H	-3.746904398	-1.481561698	2.145444461
H	-3.083354473	-3.144274232	2.687751788	H	-1.903245726	-1.873138816	4.142425149
H	-0.543091341	-2.107255224	2.547210271	H	0.390118621	-0.770139380	3.109519536
H	-5.504131812	-2.065352056	-3.575999657	H	-5.508259578	-3.651094378	-0.860695990
H	-7.435312028	-1.036809628	-1.894388169	H	-7.334024596	-1.637778622	-0.395042454
H	-5.983541251	0.442961785	-0.097815608	H	-5.750306792	0.554919973	0.084849908
H	0.441107237	0.004721742	-3.425700098	H	0.360206006	1.014029007	-3.149131683
H	-0.975692055	2.208610568	-4.265693112	H	-1.743388175	0.060389689	-4.641201141
H	-2.967798107	2.425166728	-2.404133320	H	-3.566299722	-0.719226805	-2.736062784
H	-4.645976219	2.694375220	-0.956933662	H	-3.268589675	2.357887097	-1.711435542
H	-4.969234361	4.270824613	1.256696719	H	-4.305431238	4.511150969	-0.359567932
H	-3.647127614	2.863454353	3.232594999	H	-4.457687424	3.609740214	2.245316573
C	2.283844071	-5.625528108	-2.904039193	C	5.114446357	0.305136334	4.718880271
H	3.187319975	-5.480268820	-3.501098836	F	5.779315787	-0.857288376	4.831658440
H	2.445529327	-6.478277965	-2.235953279	F	6.036746782	1.274822182	4.524420133
H	1.469434701	-5.899467400	-3.585273381	F	4.535904602	0.550701088	5.917240166
C	-0.232056452	5.139512700	3.453148519	C	5.268346422	1.015809136	-4.277887855
H	0.434317000	5.936447070	3.101548901	F	5.685270661	2.272630480	-4.506585712
H	-1.259109516	5.488972933	3.308445706	F	6.359406273	0.283238510	-3.960657667
H	-0.059199911	5.005939547	4.523809364	F	4.798385668	0.532273057	-5.451356019
C	5.497271552	1.218303498	-3.694165250	C	1.041302004	6.420688853	3.097613705
F	5.855428470	2.511166679	-3.746652231	H	1.440965757	7.137008318	2.369639474
F	6.584008084	0.516680709	-3.300888942	H	0.088239444	6.823760054	3.455677682
F	5.213623815	0.829467609	-4.958015555	H	1.735586348	6.375628653	3.940068162
C	3.762527175	-0.818992645	5.961279234	C	2.540084478	-5.616636759	-2.005671974
F	4.386491263	-1.978482882	6.222974342	H	2.590667791	-6.278284177	-1.134187113
F	4.695538221	0.157420679	6.003665894	H	1.906625436	-6.112408125	-2.750586439

F	2.901271767	-0.588191665	6.976943883	H	3.545183350	-5.524289017	-2.424495312

bor–T_4

C	1.746319501	-0.700623151	2.312041342	Ir	-0.767456376	-2.341891358	0.907520438
C	2.162901465	-2.028096103	2.439598342	C	-1.937083873	-2.080692810	2.512122169
C	2.981726723	-2.404022291	3.498733852	C	-2.115868410	-0.716780723	2.897849070
C	3.438184785	-1.485129856	4.454329479	C	-2.636826552	-3.064163630	3.223049031
C	3.016746639	-0.159100269	4.299611272	C	-1.335336745	0.265087296	2.140884796
C	2.179505075	0.268319689	3.266349079	C	-2.994708606	-0.406610068	3.945366870
C	1.681030038	1.637511387	3.077826540	C	-3.487424489	-2.704778383	4.253342507
C	1.862082812	2.723476489	3.943230069	H	-2.547755529	-4.116459564	2.978860992
C	1.274302341	3.962162987	3.676648254	C	-1.295832054	1.654489619	2.331496715
C	0.495145416	4.074243874	2.517605038	N	-0.564948741	-0.299885966	1.163845289
C	0.352603649	2.976605344	1.684133128	C	-3.696622074	-1.378108834	4.660037547
N	0.934227961	1.792353677	1.942294575	F	-3.181133204	0.888811257	4.281755343
F	3.463250585	0.723821781	5.220117633	F	-4.161232071	-3.673327407	4.898856655
F	3.331194817	-3.693904421	3.591034143	C	-0.473350219	2.461862431	1.546536769
Ir	0.719293680	0.124010210	0.709840640	H	-1.911394132	2.099303031	3.098674100
C	1.919560445	0.813588681	-0.769086911	C	0.239892853	0.467473414	0.408523138
C	2.557465172	2.060501200	-0.840891083	C	0.313616073	1.840673793	0.566580315
C	3.522200177	2.304158007	-1.806540370	H	0.823562304	-0.065233611	-0.333279709
C	3.912113846	1.331175981	-2.736906536	H	0.975391471	2.418242109	-0.071063959
C	3.266338698	0.090460730	-2.647508739	O	0.472719289	-2.414995752	-0.902386994
C	2.273966790	-0.203849164	-1.711913639	C	0.048445726	-2.240089125	-2.091623032
C	1.540903634	-1.471356623	-1.607919179	C	-1.265134467	-1.919771331	-2.489132469
C	1.633508978	-2.567866518	-2.465204740	C	-2.399813682	-1.780313505	-1.670348298
C	0.817932001	-3.689506928	-2.285583456	H	-1.419905304	-1.778996500	-3.552819195
C	-0.084995130	-3.670513956	-1.219921482	O	-2.459922745	-1.924592069	-0.402521822
C	-0.132148258	-2.571484188	-0.376772554	C	0.824116990	-2.908809729	1.988224336
N	0.670252878	-1.506190933	-0.550807890	C	1.083267198	-4.315690891	1.950924583
F	3.655812910	-0.846964226	-3.538861143	C	1.719960081	-2.093061652	2.683510182
F	4.086878186	3.522040188	-1.829823684	C	0.095987591	-5.127668905	1.233263940
B	-3.146469465	-0.203521567	-0.642690251	C	2.225285976	-4.805499312	2.589773527
N	-2.027233407	0.118268955	-1.644979833	C	2.841042211	-2.629269157	3.302402653
N	-4.242113761	0.884035901	-0.838638942	H	1.576281576	-1.020582002	2.749062226
N	-2.644783931	-0.186133309	0.855504749	C	0.112706752	-6.516806447	1.042983254

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N	-3.769054735	-1.587170825	-0.873614997	N	-0.936276330	-4.391272687	0.722297037
C	-3.507789483	-0.407932789	1.868606415	C	3.133905972	-3.999063887	3.282874072
C	-2.858298438	-0.223489432	3.078610887	F	2.505289846	-6.129362181	2.553736543
C	-1.560428159	0.125412129	2.721033520	F	3.666566786	-1.779318030	3.934962101
N	-1.418021823	0.143853317	1.377888839	C	-0.908864544	-7.159307698	0.344599960
N	-3.247255714	-2.712728286	-0.306474186	H	0.936218087	-7.089993080	1.443853470
C	-3.986154723	-3.718493551	-0.772136478	C	-1.936377887	-5.002393124	0.061166632
C	-4.993799124	-3.265601374	-1.649322437	C	-1.960914036	-6.370415949	-0.144193773
C	-4.816957049	-1.896974135	-1.684379798	H	-2.717958121	-4.344636598	-0.300870769
N	-1.766411830	-0.704053828	-2.697190894	H	-2.790678818	-6.814364812	-0.685459941
C	-0.974490781	-0.004624213	-3.508119237	C	4.344575362	-4.631578729	3.920904377
C	-0.715316892	1.288820758	-3.004945167	F	5.094153323	-3.752131338	4.608040203
C	-1.409325634	1.324680556	-1.811816146	F	3.992636133	-5.613371922	4.782826781
C	-4.514124986	1.587427713	-1.978296258	F	5.149461349	-5.200718642	2.992310104
C	-5.698299305	2.271965404	-1.783238067	C	-4.666241203	-1.100645932	5.780717621
C	-6.092715727	1.913519454	-0.476303966	F	-4.358539851	-1.821683335	6.882165101
N	-5.224863302	1.076233215	0.085409841	F	-4.696759896	0.192103204	6.152514439
H	1.853602693	-2.793782123	1.736183868	F	-5.928383152	-1.442331378	5.430476522
H	2.455350100	2.589469075	4.836753938	C	-0.411968929	3.952403917	1.761619730
H	-0.001643191	5.004762073	2.262647525	H	0.474023054	4.221124677	2.349845543
H	-0.242639130	3.019939088	0.779559566	H	-0.343512002	4.487941882	0.809575640
H	2.322336668	2.866920323	-0.156147370	H	-1.290738750	4.315387989	2.300414428
H	2.333541532	-2.534919360	-3.287960750	C	-0.879713432	-8.646849136	0.104032885
H	-0.777669943	-4.486768838	-1.050394522	H	-0.122483809	-9.139259904	0.718702468
H	-0.856313236	-2.513960081	0.425838848	H	-1.851348656	-9.102344196	0.321680018
H	-4.536801784	-0.643752481	1.651470658	H	-0.650953051	-8.861934664	-0.946911788
H	-3.270515162	-0.322656677	4.070999349	C	1.093411105	-2.428005521	-3.178220425
H	-0.716047491	0.333948096	3.359143340	H	2.101113410	-2.089741136	-2.777186873
H	-3.779089634	-4.732110908	-0.448015714	H	1.158599297	-3.551879588	-3.431493198
H	-5.745502096	-3.844390844	-2.166219703	H	0.813909664	-1.858306408	-4.130014057
H	-5.360235907	-1.126651301	-2.212253974	C	-3.725133743	-1.431632067	-2.323423427
H	-0.622489048	-0.452594815	-4.429153004	H	-3.654296403	-1.357189348	-3.410745844
H	-0.114546392	2.073325142	-3.441681851	H	-4.472334000	-2.188848321	-2.062789836
H	-1.562902177	2.127661038	-1.105765819	H	-4.086458374	-0.478179307	-1.923034288
H	-3.854461773	1.551251870	-2.833127986				
H	-6.196542459	2.932281955	-2.478420206				

H	-6.967456083	2.232999699	0.078754012
C	0.878608250	-4.849086560	-3.245040756
H	1.880869530	-4.969402413	-3.666353774
H	0.588941630	-5.785152103	-2.759793245
H	0.186344761	-4.684040722	-4.079990515
C	1.481406224	5.136158558	4.598401478
H	2.394242440	5.680579022	4.326406091
H	0.647892736	5.841397386	4.538971356
H	1.590289516	4.813679733	5.637592788
C	4.967350072	1.532025878	-3.799680078
F	5.499774626	2.764792283	-3.779317874
F	5.983435947	0.653706920	-3.647315858
F	4.456980793	1.335777929	-5.036019395
C	4.332196660	-1.831533273	5.624389477
F	4.674462733	-3.128726063	5.652977047
F	5.475811423	-1.112406255	5.589880553
F	3.721033327	-1.549320440	6.796975719

acac-T_1

Ir	-0.757649646	-2.328320577	0.948609107
C	-1.950779118	-2.087943419	2.515436112
C	-2.102338035	-0.672381852	2.919354498
C	-2.694865692	-3.061006646	3.176760374
C	-1.332076893	0.265716901	2.220027790
C	-3.035471832	-0.384937138	3.982287596
C	-3.579929495	-2.709085362	4.182336252
H	-2.610614056	-4.110091917	2.914985255
C	-1.257982366	1.690555588	2.398703606
N	-0.522673577	-0.323473272	1.196903546
C	-3.774354476	-1.360963220	4.609226486
F	-3.181801164	0.904821407	4.357470857
F	-4.306449194	-3.665350900	4.794435622
C	-0.436518077	2.474753792	1.633452894
H	-1.871780045	2.142055682	3.165427541
C	0.280851865	0.452686878	0.463118674
C	0.366717817	1.826459274	0.631328698

acac-T_2

Ir	-0.702070246	-2.318516467	0.758038948
C	-1.791444884	-1.796863764	2.384341006
C	-1.870574094	-0.391601836	2.611657611
C	-2.517955052	-2.648789119	3.223855178
C	-1.072239957	0.446059157	1.710493492
C	-2.679179696	0.091101921	3.651060607
C	-3.306006418	-2.121957816	4.232851970
H	-2.502000448	-3.725325525	3.096581505
C	-0.944127351	1.840822699	1.745379638
N	-0.382782854	-0.267668713	0.769739166
C	-3.414465480	-0.747453290	4.490823712
F	-2.764098672	1.423804840	3.852860707
F	-4.010036581	-2.963673614	5.008793524
C	-0.114344982	2.511430439	0.846918583
H	-1.496127001	2.400586725	2.485409865
C	0.429166897	0.366556001	-0.096031125
C	0.588902825	1.742622961	-0.088904069

H	0.871758376	-0.067366495	-0.283486703	H	0.947857842	-0.268748579	-0.801644699
H	1.038876771	2.397550364	-0.000079423	H	1.256980196	2.205179916	-0.808323376
O	0.459335005	-2.399020836	-0.863861791	O	0.353782134	-2.715305305	-1.031109055
C	0.026558269	-2.298959486	-2.061073563	C	0.070109667	-2.125903581	-2.185111083
C	-1.292043701	-2.014999400	-2.461577315	C	-1.194547053	-1.558994613	-2.470084503
C	-2.411657213	-1.807951691	-1.633890049	C	-2.354580873	-1.496012514	-1.658377569
H	-1.461683770	-1.935033946	-3.528812009	H	-1.318943153	-1.189081994	-3.485827084
O	-2.449970110	-1.877540808	-0.359603159	O	-2.412703069	-2.087518135	-0.473494540
C	0.841705277	-2.910024040	2.008887778	C	0.912294660	-2.824296644	1.863755126
C	1.099248836	-4.314712891	1.953628088	C	1.069661536	-4.233483792	2.041880606
C	1.748753461	-2.089016843	2.682834710	C	1.875379855	-1.974449532	2.413759892
C	0.108575488	-5.126052239	1.236059029	C	0.023225654	-5.074574622	1.453861651
C	2.257756671	-4.801046354	2.563795789	C	2.185270243	-4.697187248	2.743979038
C	2.886443858	-2.624552727	3.272791201	C	2.965460551	-2.485320041	3.104980957
H	1.598429081	-1.018075607	2.749626013	H	1.803864381	-0.897175557	2.315999959
C	0.134894971	-6.513098919	1.034605498	C	-0.039604581	-6.475369945	1.443848561
N	-0.929112374	-4.394262730	0.735044704	N	-0.974724049	-4.357308203	0.859254186
C	3.181443127	-3.993076400	3.234756709	C	3.161434307	-3.859814708	3.292600285
F	2.542152451	-6.122942454	2.516977958	F	2.364892322	-6.025880145	2.924931991
F	3.723187823	-1.778433257	3.891671413	F	3.853952441	-1.608927748	3.600243132
C	-0.883206883	-7.154341307	0.329178198	C	-1.100205372	-7.140666611	0.830530350
H	0.960382476	-7.086905179	1.430306551	H	0.755443123	-7.040111870	1.909094547
C	-1.922549354	-5.001556683	0.064543920	C	-2.010114454	-4.983765156	0.271979965
C	-1.937475121	-6.368268327	-0.156886221	C	-2.109558804	-6.363430981	0.242448011
H	-2.711267262	-4.347427329	-0.288302588	H	-2.744697305	-4.327807521	-0.182457022
H	-2.762404261	-6.813040061	-0.704377650	H	-2.960264036	-6.827025432	-0.247099393
C	4.410061771	-4.629332025	3.838285315	C	4.326226156	-4.473007000	4.029813606
F	5.195392811	-3.746484098	4.477272376	F	5.183556294	-3.554805612	4.508144791
F	4.078906506	-5.589620625	4.731086629	F	3.908107069	-5.214781148	5.081228109
F	5.168594588	-5.224761951	2.888758779	F	5.035027545	-5.300411543	3.227268983
C	-4.784739208	-1.108995132	5.706594274	C	-4.310878875	-0.285557722	5.614309512
F	-4.459924265	-1.793599624	6.826359763	F	-3.966909239	-0.872742096	6.782586539
F	-4.896940081	0.184703197	6.051624378	F	-4.274486957	1.044154940	5.813968889
F	-6.013737430	-1.528062179	5.327013454	F	-5.600091017	-0.616207056	5.374178200
C	-0.352905110	3.966962396	1.808595206	C	0.040588446	4.009209772	0.905225566
H	0.674732325	4.284419853	2.027759822	H	0.983599880	4.279804096	1.395657215

H	-0.656692052	4.491592390	0.893150723	H	0.059738779	4.445835757	-0.098121173
H	-0.994767546	4.310858330	2.623807397	H	-0.772321477	4.473140530	1.469300187
C	-0.847714992	-8.640500484	0.080577051	C	-1.153430001	-8.645840284	0.773262464
H	-0.086348802	-9.132728502	0.689999553	H	-0.410317458	-9.101185718	1.431972967
H	-1.816538330	-9.100995872	0.299743024	H	-2.143028243	-9.017809040	1.058418435
H	-0.622249489	-8.849003986	-0.972272258	H	-0.958758117	-8.997536131	-0.247221273
C	1.072478244	-2.534319654	-3.134745364	C	1.156292913	-2.190662220	-3.227460410
H	2.044921224	-2.035963204	-2.812809738	H	2.097980022	-1.774908545	-2.843985791
H	1.261606673	-3.671136812	-3.212563168	H	1.371512034	-3.229850095	-3.513716572
H	0.727862620	-2.146210969	-4.151748348	H	0.883148407	-1.640079134	-4.133034197
C	-3.739912028	-1.469710644	-2.284142075	C	-3.644392193	-0.903448831	-2.158386019
H	-3.693473097	-1.489665371	-3.375038590	H	-3.528760757	-0.459678373	-3.151934513
H	-4.505928907	-2.173315629	-1.941791002	H	-4.436133151	-1.664252370	-2.213328392
H	-4.056462824	-0.472675575	-1.959378266	H	-4.008755473	-0.123095402	-1.476995889

acac-TS$_1$

Ir	-1.000673070	-2.280847064	1.003148487
C	-2.251857677	-2.173887317	2.581701827
C	-2.346308868	-0.864807269	3.145746286
C	-3.056055740	-3.195711010	3.101512769
C	-1.456847043	0.148157334	2.585942549
C	-3.269484985	-0.639972360	4.177427381
C	-3.942898722	-2.921075568	4.128124913
H	-3.009070207	-4.208802343	2.719597068
C	-1.081512118	1.354541297	3.180280377
N	-0.901244276	-0.230486175	1.365580460
C	-4.091035550	-1.643821777	4.693128770
F	-3.380614312	0.607232060	4.682991150
F	-4.704104451	-3.921207712	4.615746603
C	-0.152967470	2.208281941	2.581703967
H	-1.519664383	1.623107865	4.132146991
C	0.035928978	0.588489941	0.798170960
C	0.414808919	1.784978484	1.354438867
H	0.449934773	0.234041035	-0.138002232
H	1.138664618	2.406041210	0.834666429
O	0.324361643	-2.194089700	-0.750509125

acac-TS$_2$

Ir	-0.655028947	-2.396087580	0.886534612
C	-2.188780318	-2.068831134	2.133439285
C	-2.294369029	-0.703202376	2.576510798
C	-3.047130617	-3.035604228	2.693510921
C	-1.402290061	0.249918554	1.939378608
C	-3.233196731	-0.394749462	3.575563453
C	-3.974490885	-2.663803268	3.640963384
H	-3.015599676	-4.073280083	2.381449603
C	-1.368007166	1.644535086	2.113413974
N	-0.523095497	-0.342219047	1.060258819
C	-4.103105127	-1.339096131	4.116885813
F	-3.305225296	0.874462345	4.031476304
F	-4.821459297	-3.587712589	4.133781041
C	-0.472948379	2.438675284	1.406734966
H	-2.059900071	2.101981511	2.805520932
C	0.354437641	0.422623050	0.377528557
C	0.410370525	1.794699728	0.515247266
H	1.022739475	-0.116285768	-0.283205251
H	1.136676109	2.359789640	-0.060309191
O	0.430829912	-2.538309659	-1.022222957

C	0.020244613	-1.911463683	-1.953285557	C	0.205209876	-1.979414766	-2.158074544
C	-1.257461781	-1.566984863	-2.443756345	C	-1.012321602	-1.450414712	-2.589861554
C	-2.456894022	-1.573792726	-1.720343627	C	-2.230909515	-1.549483355	-1.878234409
H	-1.321122126	-1.297087548	-3.491017613	H	-1.036438119	-0.990519601	-3.570817292
O	-2.604213450	-1.933607921	-0.498864104	O	-2.370738381	-2.096875518	-0.742062069
C	0.557200839	-3.272493656	1.856198409	C	0.988534324	-2.944710361	1.924641868
C	0.644433820	-4.676586070	1.665995489	C	1.113406491	-4.363297330	2.099442335
C	1.567178291	-2.606589888	2.551778653	C	1.911722319	-2.099369220	2.555687862
C	-0.440537338	-5.307062933	0.898501378	C	0.141546708	-5.188667200	1.383614608
C	1.749862368	-5.339747664	2.207102680	C	2.148960710	-4.837444306	2.907447502
C	2.638639135	-3.317197332	3.080399485	C	2.938335293	-2.626297055	3.323708690
H	1.548245518	-1.531507087	2.697211159	H	1.859909011	-1.021410988	2.447771080
C	-0.542558824	-6.663988538	0.557123142	C	0.127009804	-6.586632916	1.274663530
N	-1.411355629	-4.437967952	0.517742870	N	-0.815496492	-4.451914023	0.741129270
C	2.766266607	-4.702952917	2.926503534	C	3.086934226	-4.008365417	3.532035945
F	1.880834566	-6.676569053	2.047442112	F	2.288551154	-6.166201381	3.116820645
F	3.577039884	-2.626782548	3.744200572	F	3.820746193	-1.770239326	3.864594568
C	-1.638908536	-7.136136194	-0.163910493	C	-0.835532612	-7.234303300	0.502606515
H	0.239150635	-7.347251091	0.855411678	H	0.884944025	-7.161297249	1.787927489
C	-2.476988051	-4.881215869	-0.164780996	C	-1.746905749	-5.063754672	-0.014111528
C	-2.630919598	-6.212116333	-0.521174219	C	-1.790187071	-6.439146089	-0.154610362
H	-3.207419741	-4.123229615	-0.424015986	H	-2.454247759	-4.399658435	-0.499011597
H	-3.513764912	-6.522763822	-1.071901829	H	-2.563257959	-6.887650682	-0.770747832
C	3.911054855	-5.529452132	3.462223133	C	4.178187703	-4.638433289	4.364666868
F	4.802588306	-4.800139890	4.153365358	F	4.998854932	-3.733399071	4.923149012
F	3.465921548	-6.505166400	4.286061027	F	3.660533131	-5.382480580	5.367768836
F	4.583818327	-6.139339537	2.459359702	F	4.944189256	-5.465929156	3.617012503
C	-5.110264344	-1.449944866	5.788950077	C	-5.157072770	-1.049256967	5.158317708
F	-4.811300363	-2.203247224	6.871992928	F	-4.937126690	-1.761320012	6.286460093
F	-5.208623010	-0.176350575	6.208841592	F	-5.219421280	0.245695567	5.513798520
F	-6.342783214	-1.828395178	5.377550794	F	-6.384901228	-1.396351698	4.708361155
C	0.254527854	3.510097584	3.217080274	C	-0.439000828	3.934907003	1.581384267
H	1.313137400	3.500287280	3.507542190	H	0.543542687	4.267197839	1.937204551
H	0.124843945	4.348999661	2.521945293	H	-0.624353695	4.446713822	0.629492145
H	-0.335646578	3.719870591	4.113114573	H	-1.190553419	4.272275722	2.299473022
C	-1.750640475	-8.587204012	-0.556311701	C	-0.849817277	-8.734187763	0.356109920

H	-0.983864101	-9.195491783	-0.070769772	H	-0.099640971	-9.208825079	0.993086732
H	-2.732366183	-8.993026157	-0.290317603	H	-1.831398425	-9.144973968	0.617956387
H	-1.636784708	-8.703537750	-1.640722124	H	-0.646795346	-9.025102643	-0.681590550
C	1.183978638	-1.948645437	-2.926250375	C	1.409541649	-1.932281305	-3.080272799
H	2.005014142	-1.335655715	-2.541352246	H	2.242125076	-1.421872108	-2.583550907
H	1.559192505	-2.975503153	-2.998717156	H	1.745242790	-2.953066050	-3.293675232
H	0.909896757	-1.601980468	-3.924834051	H	1.189550187	-1.426948639	-4.023543967
C	-3.739149952	-1.148568350	-2.407859270	C	-3.490818195	-0.974087458	-2.501839940
H	-3.580118798	-0.864127966	-3.450204558	H	-3.344314429	-0.659402821	-3.538073930
H	-4.469904145	-1.963479385	-2.364649093	H	-4.294090084	-1.716511942	-2.458427812
H	-4.172811577	-0.301328594	-1.866265760	H	-3.822277096	-0.109837385	-1.914383028

acac-T_3

Ir	-0.807404818	-2.199510055	1.094899668
C	-1.989670750	-1.971902213	2.714185056
C	-2.247379141	-0.631564584	3.140678168
C	-2.652413572	-3.017722580	3.371466560
C	-1.532593318	0.455647014	2.446623089
C	-3.173436566	-0.417571190	4.175342809
C	-3.547382179	-2.749507819	4.390809131
H	-2.498223378	-4.049644858	3.077741013
C	-1.503038910	1.811920739	2.816840624
N	-0.818586982	0.053831316	1.362952891
C	-3.839947956	-1.451135727	4.833910435
F	-3.454424119	0.850693520	4.549344215
F	-4.178819164	-3.775366803	4.990284646
C	-0.757353366	2.737710391	2.086825046
H	-2.057511946	2.140837588	3.682628620
C	-0.090516743	0.930984431	0.657214623
C	-0.033037427	2.277674992	0.975442782
H	0.456253315	0.515201634	-0.183978531
H	0.564841310	2.954995475	0.373496365
O	0.431827944	-2.217841650	-0.690996825
C	0.026812915	-1.994903977	-1.875131037
C	-1.286746272	-1.654352339	-2.271483909
C	-2.425041543	-1.528124498	-1.461931987

acac-T_4

Ir	-0.720625647	-2.345085769	1.020484350
C	-2.310605862	-1.983160013	2.210057102
C	-2.406247698	-0.623002574	2.652501569
C	-3.197020628	-2.931406629	2.752842622
C	-1.483740036	0.315938522	2.023288812
C	-3.350691554	-0.292047655	3.634844658
C	-4.121269346	-2.544532972	3.700387464
H	-3.185839507	-3.968852591	2.438625777
C	-1.475060918	1.712914211	2.148537173
N	-0.567710534	-0.296880721	1.208638371
C	-4.228873380	-1.226426970	4.185434031
F	-3.417479538	0.983367137	4.074606034
F	-4.980110141	-3.459195675	4.186563542
C	-0.554686799	2.490059622	1.450273965
H	-2.206349654	2.186887502	2.786192045
C	0.333187291	0.446947575	0.534682824
C	0.370535084	1.825610619	0.627145086
H	1.018770293	-0.113606075	-0.089776315
H	1.112971339	2.378324893	0.060176928
O	0.119486410	-2.285606060	-0.997568668
C	-0.238223461	-1.804622969	-2.140884660
C	-1.518109321	-1.462493993	-2.555187537
C	-2.717699638	-1.655667922	-1.806803687

H	-1.429625455	-1.460490244	-3.327885509	H	-1.615968460	-1.037555691	-3.548072815
O	-2.519430399	-1.736312897	-0.199746274	O	-2.779845362	-2.156726892	-0.658478413
C	0.428730704	-3.543279151	1.978347542	C	1.058600026	-2.952762720	1.875195922
C	0.495410256	-4.908265352	1.581561911	C	1.178620074	-4.373552618	1.967671076
C	1.364989074	-3.049761620	2.895129687	C	2.035937189	-2.149021668	2.468522700
C	-0.532300747	-5.420164588	0.646615783	C	0.127155483	-5.160955292	1.308594716
C	1.535878144	-5.677632793	2.112839686	C	2.275702915	-4.898387177	2.652284406
C	2.391928907	-3.856423493	3.369260996	C	3.117350476	-2.721279366	3.125909298
H	1.330898734	-2.023773477	3.246587765	H	1.986649128	-1.065866904	2.422796714
C	-0.606824850	-6.724023635	0.128329126	C	0.106168429	-6.549211137	1.126800959
N	-1.466768654	-4.506254886	0.306705949	N	-0.893815037	-4.399656453	0.814893051
C	2.511827174	-5.197247674	2.994018415	C	3.270563520	-4.109165014	3.243968155
F	1.647749372	-6.985045121	1.780110971	F	2.426713761	-6.237634730	2.772651507
F	3.273834014	-3.309978354	4.220420721	F	4.040263282	-1.898093915	3.648661173
C	-1.642038398	-7.084844953	-0.736029859	C	-0.934502231	-7.166026552	0.430725325
H	0.144014072	-7.454518586	0.390974643	H	0.917612951	-7.143351931	1.522063854
C	-2.474113091	-4.847019639	-0.497831848	C	-1.901464175	-4.979782167	0.137219977
C	-2.606377469	-6.118435376	-1.042236772	C	-1.956689194	-6.348183181	-0.069769203
H	-3.195736634	-4.061809005	-0.698982170	H	-2.655436068	-4.295601363	-0.237658579
H	-3.443641245	-6.348895657	-1.694599409	H	-2.792386572	-6.768963032	-0.620291725
C	3.587117954	-6.137864371	3.479526682	C	4.418798135	-4.790687123	3.949572068
F	4.481966184	-5.536455017	4.282642329	F	5.287871139	-3.922663632	4.493539775
F	3.060493198	-7.173830616	4.171869304	F	3.975700184	-5.590400898	4.945573743
F	4.277378112	-6.670399592	2.444418669	F	5.117155064	-5.575526872	3.097220272
C	-4.845526138	-1.272435547	5.943865178	C	-5.270380707	-0.926444672	5.235743166
F	-4.482436797	-1.969565439	7.044865901	F	-5.110145255	-1.719684708	6.319341046
F	-5.003402315	0.008244598	6.324228796	F	-5.240912284	0.345764735	5.670169527
F	-6.065071832	-1.730630881	5.576600213	F	-6.516616392	-1.156542071	4.762542192
C	-0.719667551	4.192262033	2.481345048	C	-0.542676941	3.991346940	1.577889588
H	0.305614628	4.510913008	2.701207441	H	0.331461783	4.326735939	2.148953031
H	-1.085663224	4.826583856	1.665917754	H	-0.489373755	4.470856081	0.594703309
H	-1.333260307	4.385394730	3.364474755	H	-1.436704296	4.356215486	2.089416243
C	-1.706836580	-8.468343510	-1.333458567	C	-0.949165381	-8.655402939	0.200575389
H	-1.201516312	-9.203271010	-0.701034529	H	-0.188195007	-9.163088232	0.797948196
H	-2.741719661	-8.791345442	-1.481221099	H	-1.925791816	-9.083443291	0.449780003
H	-1.216512640	-8.486255477	-2.314635488	H	-0.757037387	-8.884265263	-0.854644259

C	1.097862112	-2.106475142	-2.944413535	C	0.922771537	-1.630791986	-3.106400155
H	1.978851214	-1.532889795	-2.640813254	H	1.663705557	-0.942137678	-2.684571895
H	1.412152731	-3.152649192	-3.031445055	H	1.426122682	-2.593271755	-3.246702931
H	0.756673147	-1.760528527	-3.922332341	H	0.599341743	-1.252752095	-4.078831147
C	-3.730618295	-1.107119643	-2.112608082	C	-4.031079833	-1.271072188	-2.480054673
H	-3.631569349	-0.941342328	-3.187332826	H	-3.911809288	-0.431922444	-3.171501936
H	-4.493659764	-1.873252502	-1.936582336	H	-4.408709504	-2.124020011	-3.058599377
H	-4.089924840	-0.187812881	-1.638446318	H	-4.774628246	-1.024040871	-1.719435779

Table S8. Computed vibrational frequencies (cm^{-1}) of the optimized structures.

pic–S_0	15.55	20.77	25.40	27.15	28.33	28.74
	37.53	39.42	49.14	50.03	61.81	62.88
	66.01	67.96	94.63	100.41	111.36	115.59
	119.11	147.46	153.59	157.39	164.73	171.75
	182.69	188.79	193.84	198.23	202.57	209.61
	214.36	225.90	234.81	257.33	271.85	280.75
	288.97	294.93	299.04	300.08	309.30	314.86
	321.08	331.28	338.90	339.30	346.35	349.98
	419.53	423.86	428.45	433.79	434.62	438.65
	462.24	463.93	470.43	478.24	485.20	531.46
	533.19	534.50	555.51	558.53	560.29	566.39
	584.53	584.96	589.45	591.02	596.39	598.70
	613.69	621.77	657.24	686.43	690.73	693.65
	698.19	701.56	715.12	734.99	738.24	748.46
	751.46	783.49	788.52	790.92	795.54	799.45
	830.22	837.76	845.51	853.07	855.92	863.71
	875.05	878.50	915.22	917.42	925.16	930.56
	933.81	972.52	987.44	1013.93	1022.79	1023.53
	1028.75	1041.89	1046.29	1055.12	1065.15	1065.56
	1067.69	1071.68	1072.91	1085.77	1089.53	1115.41
	1153.50	1159.73	1161.68	1162.18	1176.67	1186.97
	1187.74	1188.10	1202.20	1216.20	1220.15	1226.50
	1278.16	1280.90	1290.12	1295.22	1302.39	1311.76
	1313.42	1323.14	1327.11	1331.03	1344.90	1349.31
	1350.67	1357.37	1362.64	1425.87	1425.95	1446.72
	1447.96	1461.16	1462.30	1477.79	1486.12	1489.05
	1496.82	1497.79	1505.59	1507.33	1508.15	1526.19
	1529.65	1588.78	1598.09	1603.90	1607.89	1621.27
	1651.77	1655.50	1658.67	1668.60	1671.94	1767.98
	3046.69	3046.87	3105.73	3108.34	3138.85	3142.14
	3197.53	3204.96	3207.36	3211.35	3218.36	3223.37
	3224.14	3229.06	3235.95	3240.90	3271.50	3272.64
pic–T_1	15.66	22.56	25.54	27.43	28.01	33.70
	36.46	38.69	43.27	49.28	57.69	64.64

	66.26	88.46	94.71	107.08	112.46	118.18
	130.00	140.99	152.00	156.32	161.33	167.87
	176.18	184.80	190.61	194.18	196.61	205.75
	211.41	212.73	230.11	246.14	270.36	277.24
	282.69	288.65	293.60	296.03	308.23	309.95
	312.51	319.67	325.14	333.95	339.07	345.19
	405.43	414.92	419.07	428.85	430.94	432.33
	434.58	455.93	463.80	469.58	476.79	497.18
	525.20	526.82	531.56	533.17	541.05	545.45
	552.34	558.93	566.01	583.36	584.47	587.33
	597.88	613.87	643.27	654.97	678.48	684.75
	686.36	693.84	696.90	711.10	715.63	723.76
	738.09	750.55	764.36	767.00	782.13	789.92
	797.79	829.47	839.21	844.67	847.65	862.64
	867.63	879.51	883.31	894.58	916.43	927.81
	934.94	968.94	974.69	989.09	991.05	1006.80
	1022.69	1029.64	1039.25	1046.27	1048.01	1061.85
	1064.17	1065.53	1071.52	1073.72	1086.98	1103.84
	1116.22	1148.93	1157.34	1161.69	1177.22	1187.99
	1189.95	1190.54	1192.29	1204.96	1211.79	1217.75
	1226.74	1253.38	1278.44	1293.06	1296.78	1301.49
	1308.86	1312.44	1323.30	1328.35	1333.36	1348.58
	1350.52	1353.75	1363.90	1396.35	1424.21	1426.14
	1444.70	1446.50	1456.03	1460.26	1477.95	1486.07
	1488.62	1491.21	1496.58	1496.82	1507.10	1508.08
	1518.46	1527.30	1532.01	1598.04	1600.49	1606.61
	1607.48	1621.87	1649.81	1655.04	1670.02	1769.16
	3030.46	3047.76	3080.77	3107.04	3130.50	3143.53
	3198.04	3205.49	3206.87	3209.09	3212.66	3220.82
	3222.70	3232.29	3235.85	3238.45	3260.30	3274.00
pic–T_2	12.75	20.48	22.90	26.37	29.42	29.76
	35.47	45.38	47.69	49.35	51.64	63.96
	67.47	96.14	100.42	113.29	114.55	124.84
	149.30	152.37	164.50	165.14	176.71	183.41
	183.92	193.34	198.50	200.28	210.90	214.84

	226.41	228.76	259.97	266.08	279.83	290.71
	294.11	298.32	308.77	311.95	316.50	328.64
	330.52	334.49	336.57	343.35	348.46	395.03
	416.63	419.94	428.60	430.81	435.01	458.16
	466.22	471.14	477.49	482.56	529.91	532.76
	538.54	550.27	553.05	556.56	565.49	578.75
	582.75	586.64	587.07	591.56	596.79	605.78
	610.07	611.83	624.62	628.06	658.38	684.49
	687.05	692.58	696.64	705.12	731.89	734.10
	735.22	748.24	749.38	754.07	784.91	787.51
	791.16	797.00	829.69	844.76	850.89	851.88
	856.88	873.98	881.93	912.84	920.38	922.58
	925.46	947.69	976.69	981.09	992.68	1006.90
	1019.72	1024.47	1027.33	1042.21	1049.38	1065.66
	1067.82	1069.82	1079.67	1086.95	1131.33	1131.78
	1157.89	1159.63	1162.62	1164.48	1168.94	1172.11
	1191.33	1195.26	1205.27	1216.02	1223.01	1223.61
	1233.19	1275.43	1278.76	1288.30	1297.32	1303.75
	1311.27	1316.69	1328.92	1329.42	1348.84	1350.31
	1352.45	1355.66	1365.59	1425.93	1443.86	1449.25
	1450.28	1460.62	1460.85	1474.13	1488.43	1489.88
	1495.79	1498.32	1506.50	1511.11	1519.57	1525.85
	1527.20	1534.08	1580.25	1593.44	1596.42	1605.34
	1607.73	1620.04	1650.58	1655.92	1666.82	1669.16
	2603.29	2644.30	2735.21	3048.41	3111.17	3140.60
	3186.91	3191.95	3211.11	3213.65	3215.72	3219.67
	3221.87	3222.01	3241.10	3247.34	3266.76	3275.54
pic–TS_1	-328.56	15.68	20.10	25.59	26.23	29.82
	30.53	33.60	38.58	46.56	49.95	59.69
	62.69	65.79	70.75	83.12	89.63	99.84
	108.73	118.57	136.48	141.71	148.04	156.32
	166.40	174.03	184.74	186.37	191.97	198.81
	202.14	207.31	213.51	215.51	229.58	247.29
	254.16	265.03	279.50	286.92	292.66	297.95
	309.04	313.95	330.62	334.02	337.14	338.71

	401.54	408.64	416.37	427.86	434.49	435.69
	439.41	445.54	453.39	461.02	468.64	480.98
	526.75	529.94	531.52	532.88	535.89	539.53
	549.61	573.35	575.47	582.31	585.07	591.72
	594.34	615.21	655.65	666.94	678.87	683.97
	689.23	694.51	713.35	719.98	724.32	736.82
	745.49	755.91	771.65	778.36	780.25	786.68
	822.49	827.37	833.34	836.12	846.07	855.40
	872.92	887.05	901.13	910.36	914.79	917.10
	929.89	937.79	957.92	969.73	984.47	1010.89
	1011.44	1021.85	1027.16	1041.08	1056.35	1058.49
	1063.96	1065.11	1072.00	1073.45	1084.56	1117.93
	1136.79	1147.16	1149.08	1154.24	1178.85	1180.87
	1190.56	1192.29	1202.38	1205.74	1214.30	1224.88
	1245.17	1273.20	1273.41	1283.80	1293.08	1299.86
	1312.19	1313.09	1319.32	1326.32	1332.64	1338.46
	1341.70	1346.07	1361.62	1413.48	1424.81	1426.17
	1435.78	1436.36	1453.32	1453.56	1479.60	1480.50
	1485.91	1494.21	1496.81	1498.59	1504.28	1509.52
	1511.91	1533.15	1571.81	1590.36	1600.49	1620.21
	1620.63	1633.61	1641.14	1651.49	1654.73	1769.30
	3028.17	3045.62	3078.23	3104.33	3123.42	3140.46
	3186.61	3192.56	3199.76	3204.92	3207.82	3215.93
	3218.43	3223.29	3230.08	3230.87	3235.38	3266.82
pic–TS_2	-60.26	14.60	21.78	23.25	26.21	28.19
	30.05	33.32	36.17	47.65	50.06	59.72
	62.37	67.67	89.15	93.47	94.72	103.76
	109.72	111.99	134.84	141.22	148.03	159.31
	169.16	172.70	182.72	187.08	189.61	198.97
	203.39	208.78	222.36	226.25	257.42	273.04
	278.67	283.55	287.19	298.84	306.44	308.82
	313.67	325.14	334.09	336.50	340.41	345.53
	406.96	416.27	418.17	419.85	421.24	425.01
	447.67	455.70	457.67	459.30	470.69	520.59
	528.28	531.53	532.46	536.58	554.89	559.17

	563.50	570.87	573.96	578.93	583.52	587.63
	594.37	600.37	640.75	650.32	664.49	681.91
	690.49	695.74	706.73	719.37	727.34	736.21
	743.98	753.77	771.77	779.32	783.84	786.60
	825.77	830.59	837.09	838.07	845.82	852.65
	868.92	879.85	906.29	914.88	916.44	922.75
	934.77	977.65	991.01	991.51	1014.95	1020.62
	1025.68	1027.24	1029.24	1049.48	1058.02	1063.57
	1064.58	1067.86	1070.76	1075.93	1085.53	1115.61
	1119.08	1144.08	1160.64	1162.91	1174.83	1183.15
	1187.84	1191.55	1200.48	1207.36	1212.53	1226.16
	1264.49	1272.83	1275.41	1287.67	1298.95	1304.64
	1312.90	1320.97	1323.78	1326.18	1339.75	1344.10
	1350.53	1358.05	1359.91	1398.03	1425.74	1426.29
	1437.57	1454.73	1456.91	1464.76	1474.39	1477.07
	1494.09	1495.89	1499.18	1504.67	1507.20	1508.93
	1522.68	1538.16	1555.73	1582.91	1592.50	1606.92
	1626.63	1629.49	1641.34	1647.55	1661.73	1757.58
	3037.72	3045.76	3091.23	3103.83	3133.50	3141.92
	3194.01	3200.68	3204.77	3205.96	3214.42	3217.01
	3224.67	3227.88	3235.15	3240.40	3262.22	3266.87
pic–T_3	15.97	19.59	21.54	23.91	26.50	29.03
	32.91	36.43	40.78	45.60	46.96	54.71
	60.92	66.93	72.15	81.94	94.21	103.48
	111.21	123.50	136.64	145.02	152.14	154.70
	164.53	183.30	186.90	196.44	200.76	202.51
	209.57	212.03	212.93	227.88	236.06	249.28
	261.89	274.92	279.25	286.19	290.06	292.09
	311.48	321.86	336.07	337.55	339.01	339.75
	405.69	407.64	420.71	426.22	429.16	437.57
	451.88	457.79	463.28	466.06	471.41	530.75
	531.68	532.27	535.99	544.51	549.62	553.06
	574.17	580.24	582.62	585.46	591.67	596.39
	609.27	614.24	656.35	681.22	682.98	684.80
	691.84	699.22	705.90	733.71	736.73	745.10

	745.51	779.92	782.81	785.33	787.49	788.77
	830.26	831.73	837.52	839.19	853.47	855.81
	865.06	879.32	907.53	911.44	916.44	922.67
	935.14	973.75	991.77	1013.11	1018.43	1021.70
	1023.21	1026.20	1028.12	1041.82	1065.07	1065.76
	1067.39	1071.41	1074.79	1087.05	1089.89	1117.64
	1148.88	1154.60	1157.62	1162.21	1178.39	1187.09
	1187.73	1189.62	1202.52	1218.08	1221.35	1225.25
	1276.74	1280.92	1291.71	1294.58	1304.83	1315.43
	1318.70	1322.33	1324.92	1331.52	1339.88	1346.05
	1350.31	1353.12	1359.87	1425.85	1425.98	1433.49
	1440.13	1446.43	1454.42	1479.89	1484.56	1487.70
	1496.76	1497.38	1505.56	1505.72	1510.37	1519.94
	1524.11	1594.35	1601.63	1610.85	1616.68	1622.61
	1645.93	1650.86	1654.36	1656.67	1662.29	1755.25
	3046.65	3047.31	3105.56	3105.75	3136.25	3142.11
	3197.88	3198.21	3198.43	3198.52	3212.80	3214.02
	3225.42	3225.45	3230.83	3235.87	3277.25	3280.67
pic–T_4	13.66	16.30	22.69	25.35	28.09	28.83
	32.52	33.27	43.78	48.13	49.93	58.32
	61.63	63.52	67.61	69.33	91.19	98.78
	109.94	113.08	131.87	142.80	148.34	155.67
	160.71	165.88	181.28	186.13	190.80	199.30
	205.10	209.53	213.97	224.87	252.75	272.86
	279.42	283.05	286.38	299.91	304.36	310.47
	315.87	326.95	335.05	336.44	343.56	347.93
	407.82	412.68	416.65	420.52	421.90	425.93
	444.70	456.51	458.99	469.69	477.94	526.18
	531.13	531.84	537.74	545.56	559.23	562.67
	575.24	580.42	584.38	586.50	590.36	593.15
	597.04	607.69	637.17	666.65	674.53	685.14
	688.77	698.92	705.30	730.74	736.34	738.03
	749.36	769.71	776.96	780.88	781.66	791.08
	832.25	834.95	838.64	844.18	845.57	846.45
	871.34	880.00	913.65	917.21	920.13	921.32

	934.63	985.73	989.16	989.43	1019.02	1019.74
	1021.86	1025.72	1044.62	1053.38	1063.39	1065.14
	1065.16	1067.62	1068.97	1082.64	1087.57	1114.53
	1138.56	1149.65	1158.75	1161.37	1171.83	1183.60
	1185.77	1191.24	1201.36	1214.74	1216.07	1225.46
	1272.16	1276.13	1284.80	1291.77	1302.61	1310.21
	1311.73	1321.29	1324.16	1326.37	1340.36	1343.69
	1353.07	1361.64	1362.71	1425.68	1425.88	1435.98
	1440.90	1453.32	1458.67	1471.70	1476.32	1482.03
	1495.06	1496.14	1505.45	1506.59	1509.18	1518.15
	1526.21	1569.04	1587.34	1595.57	1604.70	1628.18
	1633.13	1639.60	1642.33	1663.36	1668.76	1744.98
	3045.08	3047.46	3101.98	3106.57	3137.52	3142.38
	3177.46	3192.62	3205.43	3206.58	3209.24	3210.83
	3214.69	3235.44	3235.75	3241.30	3267.32	3267.62
bor–S_0	16.87	20.07	23.39	23.95	27.38	30.07
	30.92	35.74	40.03	46.41	49.65	52.07
	55.86	56.34	60.67	67.62	68.76	72.03
	74.89	85.16	88.16	97.09	100.23	109.99
	115.05	120.30	139.32	151.32	154.19	159.08
	163.50	175.11	186.05	195.52	198.93	200.58
	201.44	212.47	228.51	229.75	235.60	244.17
	251.63	268.50	274.04	283.80	287.07	290.79
	295.54	306.27	308.53	314.22	316.30	318.83
	332.30	333.26	337.26	338.58	347.14	349.92
	351.13	357.05	380.16	419.64	421.15	432.68
	436.67	461.01	463.18	479.37	481.37	530.59
	532.11	553.69	555.56	558.10	563.96	579.76
	582.66	589.12	590.04	594.44	596.45	615.83
	622.45	628.48	631.35	634.40	639.12	673.43
	685.03	687.20	689.64	691.53	693.04	694.81
	698.63	725.91	737.00	747.49	749.80	773.18
	775.57	776.04	777.18	781.73	788.30	793.75
	796.42	832.71	841.11	844.60	846.52	848.52
	849.10	852.47	857.89	858.21	873.09	876.31

	878.42	881.09	889.13	893.72	901.30	905.30
	913.89	915.10	917.55	922.35	932.51	934.03
	935.80	936.41	979.08	979.65	991.15	996.16
	1010.42	1020.28	1023.36	1023.76	1037.70	1051.84
	1064.70	1065.54	1069.26	1069.70	1070.43	1074.64
	1079.27	1085.38	1097.23	1104.80	1108.24	1120.77
	1133.77	1140.27	1153.78	1159.00	1160.71	1163.02
	1187.79	1189.82	1215.15	1217.35	1217.56	1220.78
	1222.92	1223.34	1224.58	1232.64	1240.32	1245.25
	1249.12	1255.48	1273.80	1276.89	1286.21	1289.49
	1309.91	1314.52	1328.58	1329.10	1330.96	1337.14
	1340.83	1346.64	1347.71	1349.28	1358.21	1360.17
	1425.21	1425.46	1433.73	1436.20	1440.33	1444.61
	1446.33	1452.90	1456.24	1457.27	1458.41	1461.94
	1483.12	1486.47	1489.10	1489.31	1499.94	1500.78
	1504.52	1505.10	1523.80	1526.76	1564.33	1565.62
	1569.87	1572.33	1600.05	1601.13	1608.11	1609.11
	1649.71	1656.83	1668.76	1669.35	3045.64	3046.94
	3108.85	3110.06	3136.95	3138.64	3212.02	3215.00
	3219.11	3221.56	3238.18	3240.11	3255.35	3257.33
	3260.88	3269.83	3271.76	3271.96	3277.61	3278.56
	3279.81	3289.66	3291.91	3294.57	3306.47	3309.08
bor–T_1	13.37	21.84	23.38	25.67	28.12	29.60
	30.12	31.71	39.32	42.24	47.86	51.79
	53.19	60.74	63.15	68.57	70.45	75.79
	80.10	86.46	89.63	100.02	108.27	115.39
	119.70	131.96	143.11	151.24	155.70	162.02
	162.09	174.98	185.01	189.25	196.23	198.47
	200.50	209.53	222.28	226.99	233.77	242.40
	249.46	262.24	273.82	280.39	285.01	289.88
	296.04	302.97	308.13	309.42	313.56	315.48
	318.71	331.45	333.79	338.40	338.62	347.31
	349.54	354.47	378.64	404.91	414.76	420.78
	433.03	438.82	457.79	463.79	479.33	485.80
	525.08	532.42	533.32	539.91	544.64	554.39

	556.08	564.98	583.37	584.04	589.16	597.89
	617.40	628.41	631.25	634.44	639.44	640.54
	673.66	677.04	680.45	685.85	689.39	690.60
	693.28	695.36	708.31	724.98	738.19	746.79
	749.97	751.38	773.09	776.41	777.70	782.90
	789.65	794.58	832.26	840.38	844.98	845.48
	847.52	852.39	857.98	858.16	874.05	874.61
	877.90	879.41	881.63	886.08	889.70	894.63
	902.61	909.35	915.90	924.32	932.47	934.15
	935.48	937.35	951.10	955.22	979.71	990.81
	995.70	1004.83	1008.85	1021.02	1024.94	1048.45
	1052.11	1060.78	1064.14	1064.93	1069.69	1072.43
	1074.53	1086.64	1096.98	1105.15	1108.03	1114.22
	1120.85	1132.85	1139.03	1140.96	1159.10	1161.20
	1171.75	1190.54	1192.91	1193.74	1216.68	1217.85
	1220.28	1222.16	1223.51	1225.18	1232.17	1235.98
	1244.08	1248.49	1248.61	1257.00	1276.98	1291.60
	1295.63	1304.28	1315.41	1329.24	1331.41	1336.10
	1336.92	1340.62	1347.23	1349.18	1354.57	1359.96
	1405.78	1420.39	1425.50	1430.10	1434.01	1436.12
	1438.00	1439.79	1446.45	1452.01	1458.03	1459.37
	1462.00	1477.45	1484.32	1488.78	1489.78	1490.25
	1500.94	1504.15	1504.92	1526.51	1528.42	1543.91
	1563.92	1565.84	1570.06	1572.82	1587.62	1601.33
	1609.89	1633.95	1652.91	1670.29	3028.09	3046.37
	3078.38	3109.68	3131.66	3138.01	3210.66	3215.79
	3219.29	3224.14	3239.70	3240.63	3242.46	3258.79
	3260.43	3265.14	3270.23	3270.43	3277.42	3278.34
	3280.76	3289.19	3290.87	3295.25	3306.47	3310.02
bor–TS$_1$	-351.14	15.73	16.96	24.02	24.35	25.98
	29.53	30.90	34.49	40.66	46.01	48.24
	52.58	58.98	60.45	64.80	67.77	70.37
	72.60	82.34	84.96	87.43	88.84	96.39
	100.70	102.40	114.86	129.21	145.60	146.93
	156.92	165.98	173.12	186.02	188.75	193.79

197.31	200.67	206.63	216.60	224.25	224.68
239.02	241.32	245.52	256.73	271.46	273.27
275.41	282.06	290.02	292.05	295.72	311.97
328.16	329.20	329.35	332.17	333.79	339.19
349.39	353.08	378.56	399.45	408.16	410.62
429.20	433.19	452.15	456.11	459.43	483.48
530.01	530.75	542.04	543.83	547.65	552.34
571.27	575.04	580.48	585.28	590.06	603.36
611.80	621.82	630.34	633.72	636.65	666.56
668.12	677.16	681.41	683.53	687.58	688.25
692.62	701.39	717.64	723.75	744.55	749.24
762.89	773.21	775.64	776.08	778.50	782.75
784.67	813.30	831.87	834.33	839.56	842.17
844.59	848.76	851.80	858.47	860.01	874.03
876.07	878.51	887.12	892.17	895.08	902.01
905.92	910.10	911.62	914.37	915.97	931.77
932.99	934.61	937.09	956.12	977.42	980.54
995.10	1007.76	1012.11	1018.88	1019.64	1023.61
1050.30	1053.04	1059.98	1062.68	1066.47	1069.80
1074.51	1076.83	1097.45	1102.70	1108.97	1122.06
1133.78	1139.98	1144.59	1147.51	1154.41	1161.59
1189.88	1193.48	1207.18	1212.97	1214.84	1219.25
1220.00	1222.02	1224.71	1229.19	1232.50	1238.50
1243.41	1247.38	1249.69	1269.56	1275.56	1287.41
1297.43	1312.62	1323.19	1325.43	1332.68	1335.19
1336.41	1340.13	1341.51	1345.30	1354.90	1356.41
1407.55	1423.84	1426.08	1427.82	1435.72	1436.64
1436.81	1439.68	1445.08	1446.12	1457.75	1458.73
1462.41	1482.70	1484.03	1484.94	1489.46	1490.60
1493.45	1495.94	1506.06	1522.00	1524.66	1562.89
1566.33	1568.45	1570.49	1592.27	1600.19	1609.89
1614.80	1635.89	1647.01	1661.55	3025.53	3047.67
3076.74	3105.87	3128.18	3140.23	3192.97	3206.18
3217.94	3218.37	3234.29	3236.92	3238.95	3242.95
3243.67	3262.57	3270.87	3273.49	3275.81	3280.83
3283.67	3289.63	3290.11	3300.22	3306.83	3309.66

bor–TS_2	-34.30	5.13	15.56	21.78	23.19	27.69
	28.46	29.78	32.94	42.30	48.19	49.74
	53.90	54.08	58.02	59.65	63.35	64.06
	72.39	79.00	80.69	87.92	93.59	98.73
	104.84	107.72	113.35	122.78	137.70	144.89
	151.84	156.37	168.81	174.06	178.50	186.72
	190.65	204.62	207.48	211.13	214.17	224.06
	240.82	251.91	254.13	275.56	280.32	284.62
	288.85	296.62	301.82	303.24	309.54	312.62
	316.06	317.73	328.75	333.67	337.38	341.51
	344.25	348.42	357.37	411.01	416.90	418.51
	425.62	451.72	456.76	466.40	476.00	529.02
	529.79	532.05	541.68	553.98	557.98	569.58
	575.87	576.77	579.07	587.15	588.55	595.41
	604.28	629.58	632.06	636.21	644.21	660.24
	666.48	670.37	682.28	684.54	685.26	685.50
	692.69	722.70	730.75	737.26	741.79	763.94
	764.87	767.27	770.21	775.23	777.59	778.79
	785.12	823.87	828.10	832.09	837.99	839.58
	841.34	844.30	847.26	848.10	856.08	870.26
	875.16	881.81	883.29	890.07	890.65	906.30
	906.97	908.82	915.64	916.15	926.92	930.87
	932.01	933.77	971.51	981.64	986.20	990.13
	996.66	1008.61	1019.52	1022.26	1033.11	1048.73
	1064.63	1065.07	1065.82	1066.50	1067.91	1069.58
	1074.71	1081.19	1083.11	1096.10	1106.48	1115.15
	1128.04	1132.61	1137.33	1144.18	1161.72	1162.75
	1190.14	1194.23	1206.44	1208.63	1213.07	1214.45
	1219.70	1224.50	1225.21	1229.28	1232.37	1233.78
	1238.69	1251.32	1269.36	1271.36	1281.43	1285.30
	1310.55	1312.20	1320.90	1322.07	1324.50	1328.55
	1331.18	1333.00	1341.06	1343.60	1352.27	1354.30
	1423.60	1425.31	1425.83	1429.35	1433.07	1435.32
	1438.40	1442.28	1447.78	1449.51	1456.23	1459.00
	1471.09	1474.98	1480.08	1485.57	1495.96	1497.04

	1506.31	1507.47	1519.29	1526.30	1562.68	1565.74
	1567.43	1569.16	1576.70	1591.85	1593.07	1606.01
	1623.60	1631.84	1666.56	1669.83	3046.41	3047.32
	3104.85	3108.78	3139.60	3140.60	3204.12	3207.55
	3216.73	3226.59	3237.51	3237.73	3245.23	3246.22
	3260.70	3261.87	3264.79	3266.98	3270.72	3273.30
	3276.28	3280.57	3284.24	3285.99	3296.36	3299.15
bor–T_3	13.42	17.79	18.70	20.73	21.48	27.45
	31.23	31.54	38.36	42.70	45.58	49.00
	53.99	56.57	58.79	61.88	65.47	65.78
	70.91	74.21	77.99	79.57	85.61	87.08
	90.03	104.47	115.65	122.91	131.70	143.09
	150.31	151.16	169.17	172.25	194.23	196.47
	198.22	200.46	205.14	210.26	217.75	224.38
	230.47	233.36	237.26	240.06	251.92	264.06
	274.24	275.36	283.34	290.40	292.58	311.94
	314.54	328.03	331.81	333.38	338.12	341.05
	349.42	356.23	381.71	396.41	400.49	426.23
	431.57	449.94	453.85	459.62	463.85	522.90
	525.30	529.08	534.22	547.68	554.82	557.52
	569.36	578.71	583.11	584.83	589.83	611.66
	619.15	621.80	629.38	633.82	636.97	670.18
	674.63	676.50	680.43	687.06	688.18	689.77
	692.40	705.04	720.46	744.47	746.50	758.46
	770.97	773.97	775.85	779.89	781.02	783.70
	784.48	826.79	831.82	838.54	842.23	845.86
	847.21	850.39	853.76	860.05	871.29	874.27
	881.65	886.92	889.52	891.19	895.34	898.91
	903.24	912.71	913.46	917.48	929.58	932.82
	934.40	937.93	980.49	985.26	993.80	996.65
	997.26	1011.31	1014.51	1018.28	1019.38	1020.55
	1051.76	1060.04	1065.54	1066.61	1068.59	1069.94
	1073.63	1074.81	1098.03	1103.63	1108.62	1122.02
	1135.25	1145.01	1147.27	1147.48	1149.66	1153.96
	1189.12	1190.48	1212.55	1213.29	1215.00	1218.12

	1218.94	1219.63	1221.86	1230.26	1238.15	1244.98
	1250.23	1253.98	1267.40	1269.96	1282.77	1286.57
	1311.90	1313.15	1324.11	1327.46	1330.39	1332.22
	1335.73	1336.83	1340.40	1345.98	1347.40	1351.24
	1425.24	1425.40	1427.98	1430.36	1434.01	1435.37
	1435.59	1436.69	1440.43	1449.47	1458.41	1462.30
	1478.96	1481.87	1483.19	1491.35	1496.69	1496.78
	1504.20	1504.59	1516.56	1518.06	1564.63	1565.47
	1568.29	1570.16	1596.87	1600.61	1610.71	1613.39
	1641.02	1646.93	1652.26	1656.11	3046.27	3046.37
	3104.94	3105.64	3137.44	3140.08	3191.32	3200.66
	3207.51	3210.60	3213.68	3223.36	3239.03	3241.16
	3262.40	3263.91	3270.38	3274.29	3278.00	3280.01
	3284.43	3290.11	3292.08	3303.15	3307.29	3310.99
bor–T_4	7.52	15.00	18.94	21.48	27.12	28.74
	31.72	34.15	35.02	45.35	48.18	53.20
	53.96	54.32	62.57	65.00	65.65	68.29
	74.11	76.95	77.73	85.00	93.36	100.56
	105.14	114.87	117.42	124.69	137.47	145.87
	152.37	153.31	169.11	173.73	182.51	187.46
	195.30	205.26	208.52	209.87	224.24	225.26
	236.66	249.92	257.67	279.27	281.85	286.44
	290.97	297.13	300.29	304.36	310.14	314.03
	316.27	320.74	328.06	331.26	334.19	344.50
	345.73	350.76	359.57	411.57	417.14	420.47
	426.11	453.90	458.20	468.04	477.40	530.00
	530.50	533.77	541.76	553.74	561.74	569.86
	577.55	580.92	582.26	589.40	591.02	596.95
	605.52	624.71	633.92	635.16	641.81	646.32
	662.79	668.45	683.77	684.55	686.30	686.80
	691.19	721.54	727.26	738.79	744.20	763.78
	766.65	767.89	770.85	772.20	774.73	778.69
	784.19	808.30	825.17	829.31	835.63	838.14
	840.95	842.68	851.87	855.08	860.11	861.28
	868.11	880.89	884.08	885.05	890.64	896.21

	904.26	906.72	915.21	920.49	927.73	931.47
	934.36	935.89	972.69	974.79	979.62	988.65
	999.23	1006.43	1022.48	1023.04	1036.91	1045.32
	1063.51	1065.33	1067.12	1068.18	1069.25	1075.38
	1076.59	1080.14	1080.97	1097.52	1105.13	1118.70
	1120.54	1141.42	1142.12	1146.68	1158.43	1161.78
	1192.16	1193.51	1210.68	1212.05	1212.93	1214.44
	1220.60	1222.21	1223.36	1223.67	1228.56	1235.78
	1245.89	1250.99	1269.46	1272.63	1279.48	1283.11
	1310.89	1314.62	1317.39	1321.60	1323.88	1324.26
	1332.02	1339.19	1341.30	1343.92	1352.35	1357.65
	1423.80	1426.21	1427.64	1430.98	1435.83	1437.76
	1438.39	1439.84	1448.98	1449.20	1455.08	1459.36
	1465.86	1479.73	1481.89	1492.06	1499.53	1500.36
	1501.88	1504.88	1517.06	1521.24	1562.35	1566.93
	1568.43	1570.74	1590.30	1593.22	1601.76	1603.93
	1631.17	1636.27	1665.30	1668.76	3046.04	3047.02
	3109.62	3111.35	3137.27	3140.37	3211.04	3214.25
	3223.64	3224.52	3227.86	3229.17	3236.97	3239.25
	3254.68	3261.61	3263.62	3264.05	3265.59	3265.74
	3280.18	3280.32	3281.90	3282.51	3297.13	3316.47
acac-S_0	18.44	23.55	26.80	27.42	30.14	35.33
	45.54	47.18	50.15	54.55	56.31	64.07
	68.20	69.02	89.16	95.79	98.61	110.34
	116.50	150.35	153.25	158.47	162.29	163.70
	181.55	185.38	192.02	193.52	201.53	207.05
	210.09	213.17	228.07	240.33	247.46	266.07
	273.43	280.67	288.39	295.17	297.04	308.01
	313.12	320.86	330.77	337.70	339.49	346.99
	347.84	418.81	420.40	424.52	426.63	435.15
	440.77	462.66	463.77	476.92	483.99	531.90
	532.74	553.26	558.37	559.68	565.30	582.95
	584.19	588.65	589.92	591.80	595.07	596.85
	598.17	609.30	613.58	620.84	676.94	687.44
	691.06	693.26	703.05	714.01	735.28	735.95

	748.92	752.37	787.77	790.93	796.19	801.18
	806.86	844.16	846.21	855.57	864.43	875.65
	879.57	912.04	916.39	923.68	930.46	947.12
	959.75	990.75	992.59	1021.70	1023.55	1044.68
	1045.94	1053.75	1055.62	1064.94	1065.60	1067.84
	1070.28	1084.69	1089.46	1132.12	1143.91	1152.45
	1158.45	1159.40	1162.59	1185.30	1188.22	1201.22
	1213.89	1220.67	1223.31	1244.65	1275.48	1280.75
	1285.78	1292.23	1295.03	1311.11	1314.61	1327.68
	1328.12	1348.33	1349.38	1357.66	1362.17	1410.04
	1425.88	1426.04	1445.45	1448.42	1461.42	1464.79
	1471.09	1476.07	1485.76	1486.18	1489.30	1497.17
	1498.68	1504.75	1506.91	1507.99	1522.50	1525.70
	1529.07	1534.00	1563.98	1592.14	1596.18	1605.49
	1606.49	1639.46	1653.00	1661.19	1669.06	1670.49
	2589.07	2677.11	2758.28	3045.70	3046.01	3051.32
	3104.81	3107.07	3114.23	3139.01	3140.61	3146.74
	3203.18	3205.05	3205.63	3220.66	3222.80	3235.82
	3236.07	3268.09	3278.33			
acac-T_1	17.89	22.73	26.70	30.16	32.94	37.83
	43.60	44.85	48.75	52.25	63.25	67.45
	68.70	82.80	87.41	97.70	108.25	113.00
	132.89	151.63	152.56	159.29	162.66	163.40
	180.05	183.24	186.11	190.07	197.92	204.77
	208.56	210.86	223.25	228.23	239.98	264.12
	272.45	276.81	282.41	289.69	295.59	306.98
	310.06	311.04	319.12	324.01	333.90	337.79
	345.94	407.13	415.23	417.31	420.61	429.03
	433.08	438.04	457.11	463.50	480.12	493.44
	523.86	529.53	532.90	543.18	545.51	554.30
	556.51	564.30	582.84	584.92	587.22	589.86
	592.19	596.25	614.62	615.91	647.46	675.07
	679.32	683.66	688.67	694.11	713.15	714.15
	729.44	736.25	750.86	753.51	759.79	787.89
	798.30	805.10	846.34	850.15	860.28	870.25

	881.69	884.42	893.56	917.15	924.15	948.34
	956.48	961.81	969.79	990.78	1006.19	1022.11
	1045.57	1046.46	1048.00	1055.24	1060.55	1064.06
	1065.71	1072.29	1085.55	1108.66	1135.99	1145.39
	1147.33	1155.52	1158.74	1184.00	1187.73	1188.63
	1201.92	1204.27	1215.56	1224.59	1244.05	1254.12
	1275.84	1286.30	1292.52	1296.00	1310.26	1313.89
	1327.76	1333.60	1346.63	1351.61	1362.74	1400.79
	1410.00	1422.92	1426.12	1443.63	1446.49	1453.50
	1460.01	1468.90	1476.99	1484.37	1485.57	1486.88
	1490.48	1496.92	1497.97	1503.33	1507.78	1515.24
	1520.76	1526.42	1532.31	1539.53	1565.02	1598.39
	1606.28	1607.43	1607.68	1635.71	1652.08	1669.25
	2580.90	2688.83	2738.97	3025.98	3047.31	3053.01
	3074.35	3106.80	3116.58	3129.58	3142.48	3148.44
	3206.20	3207.00	3211.22	3215.87	3223.82	3229.86
	3237.43	3260.59	3269.19			
acac-T_2	10.58	19.00	25.63	27.40	29.59	32.13
	45.82	48.70	50.90	52.64	54.55	58.84
	67.88	68.78	95.38	100.39	110.05	115.99
	125.19	133.82	147.27	149.60	153.88	158.04
	167.66	177.44	185.29	192.04	194.97	197.68
	204.34	214.25	215.47	226.73	243.46	249.66
	255.54	276.78	280.86	288.04	293.52	297.21
	308.18	312.49	318.59	329.21	336.76	337.95
	340.14	347.05	347.77	400.24	413.20	419.32
	422.54	428.95	433.83	461.27	462.92	474.03
	481.03	490.06	532.24	532.97	546.63	553.84
	555.23	560.69	566.02	582.24	583.33	588.76
	589.11	595.19	596.14	611.15	617.89	657.61
	684.92	688.76	693.02	696.98	733.78	735.16
	749.64	751.63	786.43	787.89	795.23	798.43
	830.55	835.15	849.94	852.64	857.88	878.10
	883.76	903.04	912.15	914.97	916.26	923.49
	926.94	966.49	1005.33	1007.85	1021.85	1023.80

	1025.07	1036.39	1041.32	1046.56	1055.22	1064.90
	1065.40	1067.66	1069.15	1085.72	1089.17	1154.07
	1158.31	1160.70	1162.52	1165.42	1187.55	1190.81
	1201.98	1214.67	1223.24	1224.10	1274.90	1279.27
	1291.64	1293.40	1295.94	1312.93	1313.54	1325.88
	1327.98	1336.62	1347.21	1351.85	1356.77	1360.92
	1368.59	1417.22	1425.77	1425.97	1426.42	1445.84
	1446.90	1460.93	1462.19	1477.59	1478.58	1486.00
	1488.80	1496.71	1497.90	1500.06	1506.01	1507.52
	1509.04	1525.86	1529.58	1557.59	1592.20	1594.87
	1604.18	1605.71	1650.37	1655.51	1668.21	1669.49
	3007.63	3010.18	3046.27	3047.15	3050.45	3052.74
	3105.26	3108.65	3113.39	3115.52	3140.04	3141.52
	3171.92	3204.62	3207.62	3220.32	3221.22	3226.23
	3255.07	3267.61	3277.19			
acac-TS$_1$	-122.95	12.14	16.47	20.54	25.16	27.85
	31.33	40.32	41.57	47.91	49.57	51.88
	61.26	66.98	72.89	78.65	86.07	94.80
	96.92	101.63	105.83	132.18	135.05	147.05
	156.63	164.69	171.17	178.73	185.50	186.58
	195.11	199.99	203.51	206.25	210.88	216.41
	233.30	242.77	252.16	255.78	273.04	279.85
	290.33	295.58	306.70	320.20	331.75	332.13
	335.53	338.28	405.25	405.94	412.74	414.24
	425.65	426.99	430.94	452.88	458.23	462.34
	513.99	530.62	531.45	539.69	545.28	545.61
	549.30	559.67	568.51	572.25	578.19	581.80
	589.03	591.79	597.38	609.22	658.09	672.15
	673.24	678.81	682.59	686.82	719.50	729.98
	734.97	748.61	758.97	773.48	780.05	784.25
	803.01	810.75	840.72	847.95	852.21	875.78
	879.60	910.12	913.05	914.66	915.86	942.75
	946.47	951.03	952.98	1001.12	1012.36	1020.44
	1024.91	1040.98	1044.62	1048.93	1055.53	1061.45
	1062.64	1065.86	1068.58	1070.68	1084.80	1146.04

	1152.27	1154.30	1158.82	1187.09	1189.54	1201.73
	1213.55	1216.62	1224.27	1234.87	1245.67	1274.27
	1281.38	1283.46	1294.15	1308.88	1315.79	1321.28
	1326.17	1342.84	1344.13	1347.73	1358.45	1408.53
	1409.75	1424.30	1426.24	1436.04	1437.47	1443.16
	1452.82	1456.30	1463.40	1484.14	1484.45	1485.00
	1487.31	1490.16	1493.12	1496.91	1497.77	1504.88
	1507.27	1521.94	1532.84	1559.62	1583.87	1598.78
	1609.93	1621.62	1625.17	1640.09	1646.66	1662.13
	3028.75	3047.20	3051.67	3053.86	3078.38	3106.17
	3115.96	3118.23	3128.27	3140.63	3148.43	3150.17
	3192.91	3199.50	3208.69	3215.97	3226.75	3230.65
	3237.15	3249.91	3269.53			
acac-TS$_2$	-45.25	16.46	21.17	25.44	26.98	30.59
	33.65	42.30	45.06	47.29	51.97	58.64
	69.53	77.81	81.97	84.47	90.05	100.49
	103.60	108.79	111.94	118.20	125.86	140.28
	156.94	158.93	164.92	171.28	179.58	187.55
	189.47	200.50	202.45	206.39	209.45	225.01
	239.09	261.30	276.08	283.02	286.72	298.26
	304.55	310.91	313.51	327.21	334.95	336.90
	341.18	346.57	390.47	408.60	414.77	416.93
	420.45	422.04	455.00	457.16	458.74	473.87
	524.13	531.00	531.22	532.40	534.37	556.98
	559.82	566.77	568.25	572.63	578.34	582.55
	583.77	588.07	592.71	599.12	642.81	660.94
	662.51	673.87	685.09	687.65	729.08	731.27
	732.96	742.82	765.93	779.00	781.64	784.09
	792.14	826.36	842.22	845.82	847.95	873.42
	877.07	908.99	913.81	916.45	918.37	935.83
	954.09	973.69	1002.51	1016.43	1019.24	1029.11
	1033.96	1038.02	1045.63	1050.22	1059.34	1061.50
	1063.59	1064.69	1065.83	1079.15	1084.28	1127.61
	1137.29	1159.61	1161.11	1186.79	1191.64	1200.72
	1206.07	1212.60	1222.21	1223.97	1267.98	1272.12

	1278.21	1279.77	1289.22	1306.89	1312.12	1322.13
	1324.67	1338.04	1344.53	1352.67	1354.53	1403.86
	1407.94	1412.28	1425.60	1426.08	1432.68	1438.70
	1454.09	1460.61	1463.95	1471.45	1482.47	1484.06
	1489.22	1494.72	1495.53	1501.02	1502.26	1504.58
	1511.98	1523.56	1550.97	1557.66	1565.01	1576.87
	1586.08	1611.41	1619.43	1624.71	1648.03	1659.53
	3039.76	3043.58	3047.07	3047.32	3094.08	3100.10
	3109.43	3112.50	3135.08	3138.74	3141.34	3143.64
	3203.70	3203.85	3212.16	3215.03	3221.55	3227.05
	3239.10	3263.54	3269.30			
acac-T_3	8.13	15.38	18.88	22.93	28.64	30.97
	37.53	44.57	46.46	49.65	52.22	55.36
	58.08	66.80	68.24	70.40	74.09	87.33
	89.85	100.42	116.70	124.85	138.68	148.02
	151.45	166.48	171.98	176.75	182.25	188.92
	194.12	200.89	206.06	207.06	211.21	221.62
	232.11	242.38	246.74	251.09	270.03	275.67
	285.97	287.04	309.26	323.35	333.25	335.33
	337.02	342.38	400.56	408.72	413.93	417.98
	427.43	431.63	451.09	458.11	458.87	463.18
	530.44	531.22	532.40	540.67	546.75	554.15
	569.17	572.20	575.40	579.04	581.19	587.12
	590.01	594.64	608.21	616.97	664.30	676.54
	679.90	684.39	686.87	695.94	733.11	736.49
	747.44	748.08	782.81	785.28	786.68	790.15
	806.37	838.31	842.98	845.97	855.67	863.19
	883.32	909.85	913.99	914.94	921.50	946.06
	948.72	975.98	991.84	1015.95	1017.69	1022.93
	1023.76	1043.66	1045.50	1048.67	1062.40	1065.18
	1065.40	1065.72	1069.59	1086.87	1087.68	1145.91
	1148.38	1156.12	1161.49	1186.72	1187.93	1199.88
	1214.03	1219.98	1221.68	1241.48	1276.01	1276.24
	1279.14	1288.47	1294.88	1313.86	1318.47	1325.71
	1327.72	1341.00	1342.09	1351.64	1354.80	1408.75

	1409.90	1425.43	1425.78	1435.15	1439.58	1443.40
	1452.96	1455.59	1482.93	1484.52	1484.98	1486.06
	1491.11	1496.18	1500.03	1502.53	1504.81	1510.04
	1519.36	1522.06	1559.01	1589.74	1601.99	1604.90
	1618.95	1633.12	1644.19	1651.43	1654.40	1660.39
	3044.97	3046.28	3051.83	3054.15	3103.52	3106.97
	3114.81	3118.94	3136.06	3139.47	3148.85	3150.34
	3194.24	3196.82	3205.88	3212.00	3212.52	3216.73
	3224.38	3271.58	3277.54			
acac-T_4	6.28	19.16	21.43	23.47	25.99	27.46
	31.20	34.27	42.08	46.55	47.49	49.75
	55.75	60.70	63.82	78.90	87.80	98.39
	102.42	110.21	113.43	117.66	133.35	139.77
	149.19	156.74	162.62	167.53	177.93	185.43
	187.38	199.51	202.79	207.42	208.52	224.07
	225.92	254.16	278.15	281.39	286.42	299.59
	303.68	310.81	314.81	327.27	334.67	336.68
	342.54	347.53	377.09	407.48	412.71	419.91
	421.66	425.14	456.06	458.47	468.53	480.54
	527.57	531.41	531.79	534.52	545.30	558.56
	560.96	562.45	574.69	580.50	582.39	585.73
	589.65	592.43	594.93	605.86	645.79	663.99
	667.00	674.81	685.19	687.39	730.49	734.75
	737.39	747.32	774.67	780.12	781.48	790.22
	791.31	834.27	840.55	843.72	854.43	872.09
	877.83	912.43	915.49	918.11	920.27	927.09
	945.90	985.34	1015.04	1020.40	1021.54	1028.22
	1039.55	1041.29	1043.16	1052.38	1058.91	1063.38
	1065.06	1065.43	1067.55	1082.95	1087.71	1139.31
	1145.68	1159.27	1160.43	1187.61	1189.67	1200.60
	1213.25	1216.28	1223.97	1224.78	1259.70	1270.16
	1276.43	1285.33	1292.81	1309.38	1311.02	1320.92
	1325.27	1342.69	1344.27	1353.83	1358.59	1395.66
	1407.77	1426.02	1426.15	1436.85	1439.42	1452.80
	1456.27	1461.06	1478.45	1479.08	1480.26	1485.36

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