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Supporting Information

Catalytic dehydrocoupling of methylamine borane using Yamashita's [Ir(PBP)] boryl complex - characterisation of a novel highly fluxional Ir tetrahydride

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1 Experimental Section

General Information

All experiments, unless otherwise stated, were performed under oxygen - and moisture-free conditions under an inert atmosphere of argon using standard Schlenk or glove box techniques. All glassware was heated three times *in vacuo* using a heat gun and cooled under argon atmosphere. Solvents and reactants were either obtained from commercial sources (table 1.) THF, dichloromethane, toluene, *n*-hexane, *n*-pentane, diethylether and benzene were dispensed from a solvent purification system (SPS) (PureSolv, Innovative Technology) into thick-walled glass Schlenk bombs equipped with Young-type Teflon valve stopcocks, cannula transferred onto activated molecular sieves (3 Å, 0.3 nm, Carl Roth) and stored under argon in a conventional Schlenk flask. Complex ^{*t*Bu}PBPIr(H)Cl(1) was synthesised following literature procedures.¹

Substance	Origin	Purification
CH ₂ Cl ₂	local trade	taken from SPS and stored over molecular sieves (3 Å)
THF	local trade	taken from SPS and stored over molecular sieves (3 Å)
benzene	local trade	dried over Na/benzophenone stored over molecular sieves (3 Å)
toluene	local trade	taken from SPS and stored over molecular sieves (3 Å)
<i>n</i> -pentane	local trade	dried over Na/benzophenone stored over molecular sieves (3 Å)
<i>n</i> -hexane	local trade	taken from SPS and stored over molecular sieves (3 Å)
CD2Cl2	euriso-top	dried over molecular sieves (3 Å), degassed (three freeze-pump-thaw cycles) and stored in glove box
CDCl₃	euriso-top	dried over molecular sieves (3 Å), degassed (three freeze-pump-thaw cycles) and stored in glove box
C6D6	euriso-top	dried over molecular sieves (3 Å), degassed (three freeze-pump-thaw cycles) and stored in glove box
toluene- <i>d</i> ₀	euriso-top	dried over molecular sieves (3 Å), degassed (three freeze-pump-thaw cycles) and stored in glove box
[Ir(COD)CI]2	sigma aldrich	

Table S 1. C	Drigin and	purification	of solvents	and reactants.
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NMR spectra

¹H, ¹H{³¹P} ¹¹B, ¹¹B{¹H}, ¹³C{¹H} and ³¹P{¹H} NMR spectra were recorded at room temperature on Bruker AV300, AV400 or Fourier300 spectrometers. All ¹H and ¹³C chemical shifts were referenced to the solvent signal. (CD₂Cl₂: $\delta_{H} = 5.32$ ppm, $\delta_{C} = 53.84$ ppm, CDCl₃: $\delta_{H} = 7.26$ ppm, $\delta_{C} = 77.16$ ppm, C_6D_6 : $\delta_{H} = 7.16$ ppm, $\delta_{C} = 128.06$ ppm, toluene-*d*e: $\delta_{H} = 7.09$ ppm, $\delta_{C} = 137.48$ ppm, DMSO-*d*6: $\delta_{H} = 2.50$ ppm, $\delta_{C} = 39.52$ ppm).

IR spectra of crystalline samples were recorded on a Bruker Alpha II FT-IR spectrometer equipped with an ATR unit at ambient temperature under argon atmosphere or on a Bruker Alpha FT-IR-spectrometer equipped with an ATR unit at ambient temperature under aerobic conditions.

Elemental analyses were obtained using a Leco TruSpec Micro CHNS analyser. V₂O₅ was used as an oxidiser for CHN analysis of Ir complexes, circumventing possible Ir carbide formation.

Melting points (uncorrected) were determined using a Mettler-Toledo MP 70 Melt at a heating rate of 5 °C/min. Clearing points are reported.

Mass spectra were recorded on a Thermo Electron MAT 95-XP sector field mass spectrometer using crystalline samples.

UV/vis spectra were recorded on a SPECORD S 600 UV/VIS spectrometer with a diode-array detector. The samples were dissolved in toluene in a 1 cm quartz cuvette with a Schlenk-Valve.

SEC analysis was done using a 1100 GPC (Agilent Technologies) with a refraction index detector at 25 °C. The measurements were performed at a constant temperature of 25 °C using three columns with a polyester copolymer network as stationary phase (PSS GRAM 1000 Å, 5 µm particle size, 8.0 × 300 mm; PSS GRAM 100 000 Å, 5 µm particle size, 8.0 × 300 mm; PSS GRAM 1 000 000 Å). Non-stabilised THF (HPLC grade) with 1 w% Bu₄NBr added was applied as the mobile phase with a flow rate of 1 mL min⁻¹. For this purpose, 1–3 mg of the sample were dissolved in 1 mL of THF. For the recording and the evaluation of the measurement the software PSS WINGPC 6®UniChrome (PSS) was used.

2 Crystallographic Details

X-ray Structure Determination

X-ray quality crystals were selected in Fomblin YR-1800 perfluoroether (Alfa Aesar) at low temperature. Diffraction data were collected at 123(2) K on a Bruker Kappa APEX II Duo diffractometer using Mo-K_{α} radiation **2** or Cu-K_{α} radiation **4**. The structures were solved by iterative (SHELXT)² or direct methods (SHELXS-97)³ and refined by full matrix least square techniques against F² (SHELXL-2014)⁴. Semi-empirical absorption corrections were applied (SA-DABS⁵ or TWINABS⁶/Bruker). The non-hydrogen atoms were refined anisotropically. The hydrogen atoms, except the hydrides, were placed into theoretical positions and were refined using the riding model. DIAMOND (Crystal Impact GbR) was used for structure representations.

For complex **4**, electron densities up to 2.2 e/Å³ are found at a distance of about 0.8 Å from the Ir centre. Therefore, in the last refinement cycles, the positions of H2Ir and H4Ir had to be fixed with restraints.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited at the Cambridge Crystallographic Data Centre. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge, CB21EZ, UK (fax: int. code + (1223) 336-033; e-mail: deposit@ccdc.cam.ac.uk

Compound	[(^{tBu} PBP)Ir(H) ₂ (CO)] (2)	[(^{tBu} PBP)Ir(H)4] (4)
Chem. Formula	C25H46BIrN2OP2, C4H8O	C24H48BIrN2P2, C7H8
Formula weight [g/mol]	727.69	721.72
Colour	red	colourless
Crystal system	orthorhombic	monoclinic
Space group	<i>P</i> bca	<i>P</i> 21/c
a [Å]	15.5170(6)	19.1126(7)
<i>b</i> [Å]	12.1309(5)	15.5043(6)
c [Å]	34.2767(13)	11.6052(4)
α [°]	90	90
β [°]	90	106.885(2)
γ [°]	90	90
V[ų]	6452.1(44)	3290.7(2)
Z	8	4
$ ho_{calcd.}$ [g/cm ³]	1.498	1.457
µ [mm ⁻¹]	4.265	8.919
<i>T</i> [K]	150(2)	150(2)
Measured reflections	103504	5445
Independent reflections	6333	5445
Reflections with $l > 2\sigma(l)$	5497	4370
Rint	0.0437	0.0855
<i>F</i> (000)	2960	1472
$R_1(R[F^2>2\sigma(F^2)])$	0.0222	0.0614
$WR_2(F^2)$	0.0483	0.1519
GooF	1.078	1.079
No. of Parameters	354	363
CCDC #	2204735	2204734

Table S 2. Crystallographic details.

3 Preparation of complexes

3.1 Synthesis of [(^{tBu}PBP)lr(H)₂(CO)] (2)



Complex **1** (132 mg, 199 µmol) was dissolved in THF (8 mL) at room temperature. The reaction mixture was degassed (one freeze-pump-thaw-cycle) and CO gas (1 atm) was added to the reaction mixture at room temperature for 30 min. During that, a colour change from yellow to bright yellow was observed. The reaction mixture was cooled to -78 °C, cold NaBEt₃H (219 µL, 219 µmol, 1.0 mol·L⁻¹ in toluene) was slowly added and the mixture was stirred for another 15 min at ambient temperature. The reaction mixture was warmed to room temperature and stirred for another 10 min at this temperature. The solvent was removed in vacuum and the residue was extracted with benzene (2x5 mL). The solvent of the extract was removed in vacuum, yielding an orange/red coloured amorphous solid, which was recrystallised from a saturated benzene solution at room temperature to yield orange crystals (75.6 mg, 115 µmol, 58%).

¹H NMR (400 MHz, CD₂Cl₂): δ –12.23 (t, *J* = 14.6 Hz, 2H, 2x Ir-*H*), 1.36 (t, *J* = 6.7 Hz, 36H, 2x PC(CH₃)₃), 3.82 (t, *J* = 2.3 Hz, 4H, 2x CH₂), 6.72–6.81 (m, 4H, Ar-*H*) ppm. ³¹P{¹H} NMR (162 MHz, CD₂Cl₂): δ 88.6 (s) ppm. ¹¹B{¹H} NMR (96 MHz, toluene-*d*₈): δ 52.7 (br s) ppm. ¹³C{¹H} NMR (101 MHz, toluene-*d*₈): 29.7 (PC(CH₃)₃), 34.9 (PC(CH₃)₃), 43.5 (CH₂), 108.7 (*m*-C_{Ar}), 118.0 (*o*-C_{Ar}), 140.8(*C*_{q-Ar}), 183.0 (*C*O) ppm. IR (ATR, 32 scans, cm⁻¹): $\tilde{\nu}$ 2037.0 cm⁻¹ (Ir-H), 1963.6 cm⁻¹ (Ir-CO), 1818.8 cm⁻¹ (Ir-H). MS (CI+, *iso*-butane) *m*/*z*(%): 654 [M-H⁺], 655 [M-H⁺].



Figure S 1. ¹H NMR spectrum (CD₂Cl₂, 400 MHz, 298 K) of complex 2.



Figure S 2. ${}^{31}P{}^{1}H$ NMR spectrum (CD₂Cl₂, 162 MHz, 298 K) of complex 2.



Figure S 3. UV/vis spectrum of complex 2+3 in THF.



Figure S 4. IR spectrum of complex 2.

3.2 Synthesis of [(^{tBu}PBP)lr(CO)] (3)

Complex **1** (135 mg, 204 µmol) was dissolved in toluene (8 mL) at room temperature. The reaction mixture was degassed (one freeze-pump-thaw-cycle) and CO gas (1 atm) was added to the reaction mixture at room temperature for 30 min. During that, a colour change from yellow to bright yellow was observed. The reaction mixture was cooled to -78 °C, cold Na-BEt₃H (224 µL, 224 µmol, 1.0 mol·L⁻¹ in toluene) was slowly added and the mixture was stirred for another 15 min at ambient temperature. The reaction mixture was warmed to room temperature and stirred for another 10 min at this temperature. The solvent was removed in vacuum and the residue was extracted with pentane (2x5 mL). The solvent of the extract was removed in vacuum, yielding a red coloured amorphous solid, which was recrystallised from a saturated benzene solution at room temperature to yield red crystals (68.1 mg, 104.2 µmol, 51%).

¹**H NMR** (300 MHz, C₆D₆): δ 1.24 (t, J = 6.6 Hz, 36 H, 2x PC(CH₃)₃), 3.99 (s, 4H, 2x CH₂), 7.03–7.08 (m, 2H, Ar-*H*), 7.15–7.18 (m, 2H, Ar-*H*) ppm. ³¹**P**{¹**H**} **NMR** (122 MHz, C₆D₆): δ 107.2 (s) ppm. ¹¹**B**{¹**H**} **NMR** (96 MHz, C₆D₆): δ 61.8 (br s) ppm. ¹³C{¹**H**} **NMR** (75 MHz, C₆D₆): δ 29.9 (t, J = 3.1 Hz, PC(CH₃)₃), 37.1 (t, J = 9.2 Hz, PC(CH₃)₃), 43.6 (t, J = 19.8 Hz CH₂), 109.8 (s, *m*-C_{Ar}), 118.7 (s, *o*-C_{Ar}), 139.9 140.8(s, *C*_{q-Ar}), 211.4 (s, CO) ppm. **IR** (ATR, 32 scans, cm⁻¹): $\tilde{\nu}$ 1912.6 cm⁻¹ (Ir–CO). **MS** (CI+, *iso*-butane) m/z (%): 655 [M+H⁺].



Figure S 5. ¹H NMR spectrum (C₆D₆, 300 MHz, 298 K) of complex 3.



Figure S 6. ³¹P{¹H} NMR spectrum (C₆D₆, 122 MHz, 298 K) of complex 3. * complex 1, # complex 2.



Figure S 7. ³¹P{¹H} NMR spectrum (CD₂Cl₂, 122 MHz, 298 K) of a mixture of complexes **2** and **3**. Top: before irradiation (λ = 320-400 nm). Bottom: after irradiation (t_{total} = 24 min). Photodissociation of CO from **3** was observed.



Figure S 8. IR spectrum of complex 3.

3.3 Stoichiometric reaction of complex 1 with H₃B·NMeH₂



Precatalyst **1** (23.0 mg, 34.7 µmol), H₃B·NMeH₂ (1.56 mg, 34.7 µmol) and NaO*t*Bu (3.51 mg, 36.5 µmol) were dissolved in toluene- d_8 (0.7 mL) in a Young-NMR-tube. The colour of the reaction mixture turns from yellow to dark brown within a few minutes. ¹H NMR monitoring of the progress of the reaction shows a broad singlet at –10.0 ppm. The reaction mixture was filtered under hydrogen atmosphere. The solvent was evaporated in a hydrogen stream to \approx 0.2 mL. After few days colourless crystals of **4** were formed and analysed by X-ray diffraction. Removing the solvent in vacuo, results in the formation of undefined reaction products.

¹**H NMR** (400 MHz, C₆D₆): δ –9.88 (br. s, 4 H), 1.19 (t, *J* = 6.8 Hz, 36 H, 2x PC(CH₃)₃), 3.56 (t, *J* = 2.3 Hz 4 H, 2x CH₂), 6.86–6.94 (m, 2H, Ar-*H*), 7.04–7.11 (m, 2H, Ar-*H*) ppm. ³¹**P**{¹**H**} **NMR** (162 MHz, C₆D₆): δ 87.7 (s) ppm. ¹¹**B NMR** (128 MHz, C₆D₆): δ 50.5 (br s) ppm. ¹³**C**{¹**H**} **NMR** (101 MHz, C₆D₆): δ 29.5 (PC(CH₃)₃), 33.3 (PC(CH₃)₃), 43.1 (CH₂), 108.5 (*m*-C_{Ar}), 118.2 (*o*-C_{Ar}), 142.2 (*C*_{q-Ar}) ppm.



Figure S 9. Top: *in situ* ¹H NMR spectrum (toluene- d_8 , 300 MHz) of the reaction of complex **1** with NaO*t*Bu and H₃B·NMeH₂ at 298 K. Bottom: *in situ* ¹H NMR spectrum (toluene- d_8 , 400 MHz) at 207 K.



Figure S 10. In situ ³¹P{¹H} NMR spectrum (toluene- d_8 , 122 MHz, 298 K) of the reaction of complex **1** with NaO*t*Bu and H₃B·NMeH₂. * complex **1**.



Figure S 11. Variable temperature ¹H NMR experiment (toluene-*d*₈, 400 MHz) of complex **4**.

Calculation of an estimated energy barrier for dynamic hydride exchange. For this estimation, the following empirical equation was used. It should be noted that the determination of the coalescence point is only a rough approximation which should be sufficient for a qualitative estimation of the calculated energies of the transition state (TS3).

$$\Delta G^{\#} = RT_{C} \left[22.96 + ln \left(\frac{T_{C}}{\delta \nu} \right) \right] \qquad \left| \frac{J}{mol} \right|$$

Equation S 1.

On the basis of the above shown variable temperature ¹H NMR experiment (Figure S 11) we estimated the coalescence temperature $T_c = 267$ K and the frequency as $\delta v_{203K} = 556$ Hz.⁷



$$\Delta G^{\#} = (8.314 J K^{-1} mol^{-1})(267 K) \left[22.96 + ln \left(\frac{267 K}{556 s^{-1}} \right) \right] = 49339 J mol^{-1} = 49.3 k J mol^{-1}$$

- - - --

Figure S 12. Variable temperature ³¹P{¹H} NMR experiment (toluene-*d*₈, 162 MHz) of complex 4.



Figure S 13. ¹H, ¹H 31 P} and ¹H 11 B} NMR spectra (toluene- d_8 , 207 K, 400 MHz) of complex 4.



Figure S 14. Estimation of the longitudinal relaxation time T_1 for the hydride ligand (-10.0 ppm) by the inversion recovery sequence of **4** in toluene- d_8 at 293 K.



Figure S 15. ¹H{³¹P} inversion recovery experiment of hydride signal (-10.0 ppm) in toluene-*d*₈ at 293 K of **4**.



Figure S 16. Estimation of the longitudinal relaxation time T_1 for the hydride ligand (-9.24 ppm) by the inversion recovery sequence of **4** in toluene- d_8 at 207 K.



Figure S 17. Estimation of the longitudinal relaxation time T_1 for the hydride ligand (-10.7 ppm) by the inversion recovery sequence of **4** in toluene- d_8 at 293 K.



Figure S 18. ¹H{³¹P} inversion recovery experiment of hydride signals (-9.24 and -10.7 ppm) in toluened₈ at 207 K of **4**.

3.4 Deuteration experiments – Reaction of complex 1 with D_3B ·NMeH₂ and NaO*t*Bu

Precatalyst **1** (35.0 mg, 45.3 μ mol), D₃B·NMeH₂ (2.17 mg, 45.3 μ mol) and NaO*t*Bu (4.57 mg, 47.6 μ mol) were dissolved in toluene-*d*₈ (0.7 mL) in a Young-NMR-tube. The colour of the reaction mixture turns from yellow to dark brown after a few minutes. ¹H NMR monitoring of the progress of the reaction shows a broad singlet at –10.0 ppm.



Figure S 19. ¹H NMR spectrum (toluene- d_8 , 400 MHz, 298 K) of the reaction of complex **1** with NaOtBu and D₃B·NMeH₂.



Figure S 20. ¹H NMR spectrum (toluene-*d*₈, 400 MHz, 203 K) of the reaction of complex **1** with NaOtBu and D₃B·NMeH₂. Hydride signals at δ -9.2 ppm, -10.7 ppm.



Figure S 21. ¹H{³¹P} NMR spectrum (toluene- d_8 , 400 MHz, 203 K) of the reaction of complex **1** with NaO*t*Bu and D₃B·NMeH₂. Hydride signals at δ -9.2 ppm, -10.7 ppm.

3.5 Deuteration experiments – Reaction of 4 with D₂

Precatalyst **1** (35.0 mg, 45.3 μ mol), H₃B·NMeH₂ (2.03 mg, 45.3 μ mol) and NaO*t*Bu (4.57 mg, 47.6 μ mol) were dissolved in toluene-*d*₈ (0.7 mL) in a Young-NMR-tube. The colour of the reaction mixture turns from yellow to dark brown after a few minutes. The reaction mixture was frozen, degassed (3x) and the H₂ atmosphere was exchanged with D₂ gas. The reaction mixture was then analysed by NMR experiments at 203 K and room temperature.



Figure S 22. ¹H NMR spectrum (toluene- d_8 , 400 MHz, 298 K) of complex **4** after gas exchange with D₂ at room temperature.



Figure S 23. ¹H{³¹P} NMR spectrum (toluene- d_8 , 400 MHz, 203 K) of complex **4** after gas exchange with D₂ at room temperature.



Figure S 24. ¹H NMR spectrum (toluene- d_8 , 400 MHz, 203 K) of complex **4** after gas exchange with D₂ at -78 °C.



Figure S 25. ¹H{³¹P} NMR spectrum (toluene- d_8 , 400 MHz, 203 K) of complex **4** after gas exchange with D₂ at -78 °C.



Figure S 26. ¹H saturation transfer experiment (toluene-*d*₈, 400 MHz, 203 K) of the gas exchange reaction with D₂ at -78° C with complex **4**, performed at the hydride signals. Top: Presaturation at -10.74 ppm. Bottom: Presaturation at -9.30 ppm. In both cases, the intensity of the other hydride signal is clearly reduced. Selectivity of the saturation was proven by irradiation at -7.68 ppm which has no effect.

3.6 Reaction of complex 1 with LiTMP and H₂

Complex **1** (24.8 mg, 34.5 µmol) and LiTMP (1.05 eq.,1.61 mg, 39.3 µmol) were dissolved in toluene- d_8 (0.7 mL) in a Young-NMR-tube. The reaction mixture was degassed (three freeze-pump-thaw-cycles). Then the reaction mixture was frozen at –196°C, evacuated, followed by purging with H₂ gas. The mixture was then allowed to slowly warm to room temperature under vigorous stirring. This H₂ purging cycle was repeated at least three times. Afterwards the reaction mixture was stirred at 90°C overnight. The colour of the reaction mixture turns from yellow to dark brown. ¹H NMR monitoring of the reaction solution shows a broad singlet at –10.1 ppm.



Figure S 27. ¹H NMR spectrum (toluene- d_8 , 300 MHz, 298 K) of the reaction of complex 1 with LiTMP and H₂. * complex 1.

87.6 85.1 85.1



Figure S 28. ³¹P{¹H} NMR spectrum (toluene- d_8 , 122 MHz, 298 K) of the reaction of complex **1** with LiTMP and H₂. * complex **1**.



3.7 Reaction of 1 (5 mol%) with H₃B·NMeH₂

Figure S 29. ¹H NMR spectrum (toluene- d_8 , 300 MHz, 298 K) of the reaction of **1** (5 mol%) with H₃B·NMeH₂.

- 76.6

- 87.6



Figure S 30. ³¹P{¹H} NMR spectrum (toluene- d_8 , 122 MHz, 298 K) of the reaction of **1** (5 mol%) with H₃B·NMeH₂.

4 Dehydrocoupling of amine boranes

4.1 General procedure

H₃B·NH₃ or H₃B·NMeH₂ (1.33 mmol), NaO*t*Bu (1 mol%) and the corresponding precatalyst (1 mol%) were weighed into a three-necked reaction vessel. The reaction vessel was connected to an automatically operating gas buret⁸ under Ar atmosphere. The gas buret was initialised, the solvent (THF or toluene, 10 mL) was added, and the data acquisition was started immediately. After the reaction, a gas sample was taken and analysed by TCD-GC to confirm the presence of H₂. An aliquot was taken from the reaction mixture and analysed by NMR spectroscopy (¹H, ³¹P{¹H}, ¹¹B, ¹¹B{¹H}).

4.2 Overview of the catalytic conditions

 entry	catalyst	<i>c</i> / mol%	substrate	solvent	reaction	equivalent
					time / h	H ₂
1	1	1.0	H ₃ B·NMeH ₂	toluene	1.25	0.85
2	1	2.0	H ₃ B·NMeH ₂	toluene	0.20	0.92
3	1	1.0	H ₃ B·NMeH ₂	THF	44.4	0.88
4	1	2.0	H ₃ B·NMeH ₂	THF	88.5	0.94
5 ^a	2	1.0	H ₃ B·NMeH ₂	toluene	25.0	0.78
6 ^a	3	1.0	H ₃ B·NMeH ₂	toluene	12.5	0.90
7 ª	3	0.1	H ₃ B·NMeH ₂	toluene	50.0	0.89
8	1	1.0	H₃B·NH₃	THF	60.0	1.03
9	1	1.0	H₃B·NH₃	toluene	93.0	0.85
10ª	2	1.0	H₃B·NH₃	THF	45.0	0.53

Table S 3. Overview of the catalytic conditions for the dehydrocoupling of amine boranes.

Reaction conditions: c(substrate) = 1.33 M, V(Solvent) = 10 mL, 1 eq. NaOtBu.^a Without the use of NaOtBu.

4.3 Dehydrocoupling of H₃B·NMeH₂



Figure S 31. Volumetric curves of the dehydrocoupling of H₃B·NMeH₂ with complex 1 and NaOtBu.



Figure S 32. ¹¹B{¹H} and ¹¹B NMR spectra (96 MHz, toluene- d_8) of dehydrocoupling of H₃B·NMeH₂ with complex **1**. Conditions: $T = 25^{\circ}$ C, toluene, 1 mol% NaO*t*Bu, 1 mol% **1**.



Figure S 33. ¹¹B{¹H} and ¹¹B NMR spectra (128 MHz, toluene- d_8) of dehydrocoupling of H₃B·NMeH₂ with complex **1**. Conditions: $T = 25^{\circ}$ C, toluene, 2 mol% NaOtBu, 2 mol% **1**.



Figure S 34. ¹H (300 MHz) and ¹¹B NMR spectra (96 MHz) in THF- d_8 of isolated (H₂B·NMeH)_n Conditions: $T = 25^{\circ}$ C, toluene, 2 mol% NaOtBu, 2 mol% **1**.



Figure S 35. SEC data of isolated polymer from the dehydropolymerisation of $H_3B \cdot NMeH_2$ with 2 mol% **1**.



Figure S 36. Volumetric curve of the dehydrocoupling of H₃B·NMeH₂ with complex 1.



Figure S 37. ¹¹B{¹H} and ¹¹B NMR spectra (96 MHz, THF-*d*₈) of dehydrocoupling of H₃B·NMeH₂ with complex **1**. Conditions: $T = 25^{\circ}$ C, THF, 1 mol% catalyst.



Figure S 38. Volumetric curves of the dehydrocoupling of H_3B ·NMeH₂ with complex 2 and 3.



Figure S 39. ¹¹B{¹H} and ¹¹B NMR spectra (96 MHz, toluene- d_8) of dehydrocoupling of H₃B·NMeH₂ with complex **3**. Conditions: $T = 25^{\circ}$ C, toluene, 1 mol% catalyst.



Figure S 40. ¹¹B{¹H} and ¹¹B NMR spectra (96 MHz, toluene- d_8) of dehydrocoupling of H₃B·NMeH₂ with complex **2**. Conditions: $T = 25^{\circ}$ C, toluene, 1 mol% catalyst.

4.4 Reactivity test of 2 for the dehydrocoupling of H₃B·NMeH₂



A mixture of complexes **2** and **3** (90:10) in CD₂Cl₂ was irradiated at 320–400 nm in a Young-NMR tube for 20 minutes. The corresponding ³¹P{¹H} NMR spectra confirmed the photo-cleavage of complex **3** (Figure S 41) in solution. Afterwards, the solvent was removed in vacuum and toluene- d_8 (0.6 mL) was added, followed by the addition of H₃B·NMeH₂ (6.0 mg). The ¹¹B and ¹¹B{¹H} revealed almost no conversion of the substrate after 12 hours (Figure S 42).



Figure S 41. ³¹P{¹H} NMR spectra (CD₂Cl₂, 122 MHz, 298 K) of a mixture of complexes **2** and **3**. Top: before irradiation (λ = 320-400 nm). Bottom: after irradiation (t_{total} = 20 min).





Figure S 42. ¹¹B and ¹¹B{¹H} NMR spectra (96 MHz, toluene- d_{3}) of dehydrocoupling of H₃B·NMeH₂ with complex **2** after photocleavage of **3**.

4.5 Dehydrocoupling of H₃B·NH₃



Figure S 43. Volumetric curves of the dehydrocoupling of $H_3B \cdot NH_3$ with complex 1.



Figure S 44. ¹¹B{¹H} and ¹¹B NMR spectra (96 MHz, THF-*d*₈) of dehydrocoupling of H₃B·NH₃ with complex **1**. Conditions: $T = 25^{\circ}$ C, THF, 1 mol% catalyst.



Figure S 45. ¹¹B{¹H} and ¹¹B NMR spectrum (96 MHz, DMSO-*d*₆) of dehydrocoupling of H₃B·NH₃ with complex **1** after work up. Conditions: $T = 25^{\circ}$ C, THF, 1 mol% catalyst.



Figure S 46. Volumetric curve of the dehydrocoupling of H₃B·NH₃ with complex 2.



Figure S 47. ¹¹B{¹H} and ¹¹B NMR spectrum (96 MHz, THF-*d*₈) of dehydrocoupling of H₃B·NH₃ with complex **2**. Conditions: $T = 25^{\circ}$ C, THF, 1 mol% catalyst.

5 Computational Details

Computations were carried out using Gaussian 16⁹. In our calculations, we have used the reasize molecules. Calculations were carried out using hybrid functional density functional method B3LYP¹⁰⁻¹⁵ in combination with basis set def2tzvp¹⁶ and the empirical dispersion correction GD3BJ^{17, 18}. All geometries were confirmed to be local minima or first order saddle points (for transition states, TS) on the potential energy surface by harmonic vibration frequency calculations on the same level of theory. Transition states were proofed to be correct by intrinsic reaction coordinate scans in both directions. For the visualisation of the charge density difference between the ground state and selected excited states as well as for QT-AIM^{19, 20} and Laplacians-Plot Analysis we used MultiWfn 3.6 employing Gaussian16 formatted checkpoint files.²¹ For the visualisation of 3D-quantum chemical results we used GaussView6.1.1²² and Avogadro^{23, 24}. In addition to the electronic supporting information we provide a multi-structure xyz-file including all calculated molecules. For a better understanding and a more intuitive view of the calculated 3D structures, we strongly recommend using this file e.g. with the free program MERCURY.²⁵

Please note that all computations were carried out for single, isolated molecules in the gas phase, if not otherwise noted (ideal gas approximation). There may well be significant differences between gas phase and condensed phase.

Comp. label	File-Name	Nimag	HF	ZPE [kcal/mol]	H _{tot} [a.u.]	G _{tot} [a.u.]	Method	Basisset	Cacl
2	t ^{Bu} PBPIr(H)₂CO	0	-1977.966957	422.412660	-1977.254478	-1977.359510	B3LYP/GD3BJ	def2tzvp	opt/freq
	t ^{Bu} PBPIr(H) ₂	0	-1864.540911	416.184820	-1863.840140	-1863.942443	B3LYP/GD3BJ	def2tzvp	opt/freq
3	t ^{Bu} PBPIr(CO)	0	-1976.761654	411.473630	-1976.066455	-1976.173802	B3LYP/GD3BJ	def2tzvp	opt/freq
int1	PBPIrH4_iso2xray_b3lyp_opt_freq_tzvp.out	0	-1865.7421097	427.42039	-1865.023388	-1865.124840	B3LYP/GD3BJ	def2tzvp	opt/freq
int3	PBPIrH4_iso1_b3lyp_opt_freq_tzvp.out	0	-1865.7405711	426.46881	-1865.022835	-1865.124493	B3LYP/GD3BJ	def2tzvp	opt/freq
int1	PBPIrH4_iso2_b3lyp_opt_freq_tzvp.out	0	-1865.7421097	427.42390	-1865.023383	-1865.124833	B3LYP/GD3BJ	def2tzvp	opt/freq
int1_1	PBPIrH4_iso2_2_opt_freq_tzvp.out	0	-1865.7421097	427.42396	-1865.023383	-1865.124834	B3LYP/GD3BJ	def2tzvp	opt/freq
int2	PBPIrH4_iso3_b3lyp_opt_freq_tzvp.out	0	-1865.7297392	426.63010	-1865.011766	-1865.113813	B3LYP/GD3BJ	def2tzvp	opt/freq
	PBPIrH4_iso3_2_b3lyp_opt_freq_tzvp.out	0	-1865.7421097	427.42203	-1865.023384	-1865.124843	B3LYP/GD3BJ	def2tzvp	opt/freq
TS5	PBPIrH4_TS1_b3lyp_opt_freq_tzvp-1.out	1	-1865.7385889	426.21145	-1865.021703	-1865.122481	B3LYP/GD3BJ	def2tzvp	opt/freq
TS4	PBPIrH4_TS2_b3lyp_opt_freq_tzvp.out	1	-1865.7338617	425.32428	-1865.018344	-1865.119321	B3LYP/GD3BJ	def2tzvp	opt/freq
	PBPIrH4_TS3_b3lyp_opt_freq_tzvp.out	1	-1865.7288988	425.52371	-1865.012970	-1865.114261	B3LYP/GD3BJ	def2tzvp	opt/freq
TS2	PBPIrH4_TS3_2_b3lyp_opt_freq_tzvp.out	1	-1865.7302877	425.51275	-1865.014429	-1865.115628	B3LYP/GD3BJ	def2tzvp	opt/freq
TS1	PBPIrH4_TS4_b3lyp_opt_freq_tzvp2.out	1	-1865.7401797	426.23189	-1865.023487	-1865.124352	B3LYP/GD3BJ	def2tzvp	opt/freq
TS3	PBPIrH4_TS5_b3lyp_opt_freq_tzvp.out	1	-1865.7219982	426.69645	-1865.00422	-1865.105651	B3LYP/GD3BJ	def2tzvp	opt/freq
TS5_Cs	PBPIrH4_TS1_Cs_b3lyp_opt_freq_tzvp.out	1	-1865.7384428	426.11433	-1865.021651	-1865.122919	B3LYP/GD3BJ	def2tzvp	opt/freq

Table S 4. Summary of thermodynamic data of all calculated compounds.





Figure S 48. Calculated (black, B3LYP/GD3BJ/def2tzvp) and experimental (red) IR spectra of complex 2.



Figure S 49. Calculated (black, B3LYP/GD3BJ/def2tzvp) and experimental (red) IR spectra of complex **2.** Experimental: \tilde{v} 2037.0 cm⁻¹(Ir–H), 1963.6 cm⁻¹(Ir–CO), 1818.8 cm⁻¹(Ir–H). Calculated: \tilde{v}_{cal} 2127 cm⁻¹ (Ir–H), \tilde{v}_{cal} 2040 cm⁻¹ (Ir–CO), \tilde{v}_{cal} 1787 cm⁻¹ (Ir–H); Note: \tilde{v} 1912.6 cm⁻¹ (Ir–CO) of **3**.

5.2 Calculated IR spectra of [(^{tBu}PBP)Ir(CO)] (3)



Figure S 50. Calculated (B3LYP/GD3BJ/def2tzvp) IR spectra of complex 3, $\tilde{v}_{calc.}$ 2001 cm⁻¹ (Ir–CO).

5.3 Calculated UV/VIS spectra of [(^{tBu}PBP)Ir(H)₂(CO)] (2)



Figure S 51. Calculated (B3LYP/GD3BJ/def2tzvp) UV/VIS spectra of complex 2 with solvent correction in THF.

5.4 Calculated UV/VIS spectra of ^{tBu}PBPIr(CO) (3)



Figure S 52. Calculated (B3LYP/GD3BJ/def2tzvp) UV/VIS spectra of complex 3 with solvent correction in THF.

Excitation energies and oscillator strengths:

Excited State 3:	Singlet-A	3.4118 eV 363.40 nm f=0.2904 <s**2>=0.000</s**2>
129 -> 135	0.10197	
133 -> 135	0.68617	
Excited State 30	: Singlet-A	5.6289 eV 220.26 nm f=0.3088 <s**2>=0.000</s**2>
129 -> 136	0.41690	
130 -> 137	-0.34891	
131 -> 137	0.20435	
131 -> 138	0.19383	
133 -> 136	0.16445	
133 -> 141	-0.16388	
133 -> 146	-0.11401	

 Table S 5. Orbital contour plot of the exited state 3 (363.4 nm) of ^{#Bu}PBPIr(CO).



5.5 Charge density difference

Table S 6. Charge density contour plot of complex **3** at the exited state 3 (363.4 nm).



5.6 Theoretical investigation of [(^{tBu}PBP)Ir(H)₄] (4)

In this chapter, we summarise the results of our DFT calculations performed at the B3LYP/GD3BJ/def2tzvp level of theory in terms of the energy difference of all isomeric structures of tetrahydride complex **4** considered. Previous studies showed that the potential energy surface of such iridium tetrahydride and/or dihydrogen/dihydride complexes is very low. Noteworthy to mention that Goldman, Krogh-Jespersen *et. al.*²⁶ revealed a slight shift of the energy surface of [(POCOP)Ir(H)₄] pincer complex when considering a solvent correction but only small differences in energy between the considered isomers were reported. This agrees well with our calculations. It should be mentioned that these small differences are below the error of the calculations and should therefore be discussed with caution. A detailed analysis of the data can be found in the manuscript.

Table S 7. Summary of calculated thermodynamic data for the *trans*-pathway of the tetrahydride dihydrogen/dihydride exchange of complex **4.**

Comp. Label	Calc. label	$\Delta_{\rm R}$ H [kJ/mol]	$\Delta_{\rm R} G [kJ/mol]$	$\Delta_{\rm R}$ H [kcal/mol]	$\Delta_{\rm R}$ G [kcal/mol]
int1_2	PBPIrH4_iso2_2_opt_freq_tzvp.out	0.0	0.0	0.0	0.0
TS1	PBPIrH4_TS4_b3lyp_opt_freq_tzvp.out	-0.3	1.3	-0.1	0.3
int1	PBPIrH4_iso2xray_b3lyp_opt_freq_tzvp.out	0.0	0.0	0.0	0.0
TS4	PBPIrH4_TS2_b3lyp_opt_freq_tzvp.out	13.2	14.5	3.2	3.5
int3	PBPIrH4_iso1_b3lyp_opt_freq_tzvp.out	1.5	0.9	0.3	0.2
TS5	PBPIrH4_TS1_Cs_b3lyp_opt_freq_tzvp.out	4.4	6.2	1.1	1.5
int3_2	PBPIrH4_iso1_b3lyp_opt_freq_tzvp.out	1.5	0.9	0.3	0.2

 Table S 8.
 Summary of calculated thermodynamic data for the *cis*-pathway of the tetrahydride dihydrogen/dihydride exchange of complex 4.

Comp. Label	Calc. label	$\Delta_{\rm R}$ H [kJ/mol]	$\Delta_{\rm R} G [kJ/mol]$	$\Delta_{\rm R}$ H [kcal/mol]	$\Delta_{\rm R}$ G [kcal/mol]
int1	PBPIrH4_iso2xray_b3lyp_opt_freq_tzvp.out	0.0	0.0	0.0	0.0
TS2	PBPIrH4_TS3_2_b3lyp_opt_freq_tzvp.out	23.5	24.2	5.6	5.8
int2	PBPIrH4_iso3_b3lyp_opt_freq_tzvp.out	30.5	29.0	7.3	6.9
TS3	PBPIrH4_TS5_b3lyp_opt_freq_tzvp.out	50.3	50.4	12.0	12.0
int2_2	PBPIrH4_iso3_b3lyp_opt_freq_tzvp.out	30.5	29.0	7.3	6.9



Figure S 53. Plot of the calculated reaction enthalpies for the iridium polyhydride system 4 (B3LYP/GD3BJ/def2tzvp).



Figure S 54. Plot of the calculated Gibbs free reaction energies for the iridium polyhydride system **4** (B3LYP/GD3BJ/def2tzvp).



Figure S 55. Contour plot of the Laplacian of the electron density $\nabla^2 r$ of Ir complex **4** in the B-Ir-H plane of **int1** structure. Dashed lines indicate negative (local charge concentration), solid lines indicate positive values (local charge depletion). The Laplacian plot is overlaid with the molecular graph from QT-AIM analysis and wiberg bond indices (italic small numbers). Brown lines indicate bond paths, blue dots correspond to bond critical points, dashed brown lines are hypothetical bond path which were drawn manually in this graph. Density from B3LYP/GD3BJ/def2tzvp calculation.



Figure S 56. Contour plot of the Laplacian of the electron density $\nabla^2 r$ of Ir complex **4** in the B-Ir-H plane of **int1_2** structure. Dashed lines indicate negative (local charge concentration), solid lines indicate positive values (local charge depletion). The Laplacian plot is overlaid with the molecular graph from QT-AIM analysis and wiberg bond indices (italic small numbers). Brown lines indicate bond paths, blue dots correspond to bond critical points, dashed brown lines are hypothetical bond path which were drawn manually in this graph. Density from B3LYP/GD3BJ/def2tzvp calculation.



Figure S 57. Contour plot of the Laplacian of the electron density $\nabla^2 r$ of Ir complex **A** in the B-Ir-H plane. Dashed lines indicate negative (local charge concentration), solid lines indicate positive values (local charge depletion). The Laplacian plot is overlaid with the molecular graph from QT-AIM analysis and wiberg bond indices (italic small numbers). Brown lines indicate bond paths, blue dots correspond to bond critical points. Density from B3LYP/GD3BJ/def2tzvp calculation.



Figure S 58. Contour plot of the Laplacian of the electron density $\nabla^2 r$ of Ir complex **B** in the B-Ir-H plane. Dashed lines indicate negative (local charge concentration), solid lines indicate positive values (local charge depletion). The Laplacian plot is overlaid with the molecular graph from QT-AIM analysis and wiberg bond indices (italic small numbers). Brown lines indicate bond paths, blue dots correspond to bond critical points. Density from B3LYP/GD3BJ/def2tzvp calculation. **Table S 9:** Summary of Natural Charge Analysis from NBO6.027-30 calculations of the literature knowncomplex **B** and the here described complex **4**.

I -0.36171 H Horidge 7.3 idge 22 -0.07261 H 7.6 idge 7.8 -0.0333 H 7.6 Sum -0.51303 P 2.3 i 3 1.17355 P 2.3 i 6 -0.50462 C 5.6 i 8 0.20161 H 7.7 i 9 -0.50444 H 8.9 i 1.0.20419 C 1.0 9.9 i 0.20230 H 1.0 1.0 i 2.2 -0.61033 H 1.0 1.0 i 3.0 0.20281 H 1.0 1.0 i 3.0 0.20281 H 1.0 1.0 i 3.0 0.20281 H 2.2 1.0 1.0 1.0 i 3.0 0.20281 H 2.2 1.0 1.0 2.2 <	 Atom	Number	Nat Charge	Atom	Number
23 -0.07121 H bdge 77 125 0.02391 H 78 Sum -0.5130 FM 77 12 1.17855 P 22 3 1.17936 P 23 6 -0.50442 C 55 7 0.20426 C 65 8 0.20161 H 99 31 10 0.20426 H 91 31 11 0.20429 H 131 91 31 23 0.20426 H 131 141 131 131 0.60753 H 151 141 131 133 0.2055 H 122 142 123 133 0.2057 H 222 124 124 124 141 0.2026 H 223 143 124 124 142 0.20673 C 124 124 124 <tr< td=""><td>Со</td><td>1</td><td>-0.36171</td><td>Ir</td><td>1</td></tr<>	Со	1	-0.36171	Ir	1
idge 24 0.0022 H 177 idge 78 0.0333 N 78 idge 78 0.0333 N 78 idge 78 0.0333 N 78 idge 78 0.0333 N N idge 1.17936 P 2 1 idge 0.020426 C 65 idge 0.20426 C 66 idge 0.20426 H 78 79 idge 0.20351 H 10 22 0.2032 idge 0.20331 C 13 16 13 idge 0.20321 H 131 16 14 12 idge 0.20325 H 14 22 23 23 0.2032 H 22 idge 0.2026 H 22 24 26 26 22 idge 0.2027 H 22 <td>Н</td> <td>23</td> <td>-0.07121</td> <td>H bridge</td> <td>75</td>	Н	23	-0.07121	H bridge	75
25 -0.12761 H 77 Sum -0.51303 Sum -0.51303 Sum Sum 2 1.17855 P 2 2 1 3 1.17936 P 2 1 7 0.20426 C 55 1 7 0.20426 C 56 1 9 -0.50444 H 89 1 10 0.20416 H 71 1 0.20419 C 100 1 0.20419 H 11 1 0.20426 H 111 1 0.20236 H 111 1 0.20236 H 111 1 0.20236 H 111 1 0.20237 H 22 1 0.20237 H 22 1 0.20327 H 24 1 0.20327 H 24 1	H bridge	24	0.0082	н	76
idge 78 0.0333 H 0.78 Sum -0.51303 P 2 3 1.17936 P 3 6 -0.50462 C 53 7 0.20426 C 56 8 0.20161 H 9 -0.50444 10 0.20161 H 9 -0.50444 11 0.20419 C 100 22 -0.61033 H 112 22 0.2032 H 113 23 0.20255 H 115 33 0.20255 H 115 33 0.20255 H 22 33 0.20257 H 22 33 0.20257 H 22 33 0.20257 H 22 44 0.20650 H 22 44 0.20257 H 28 44 0.20257 H 28	н	25	-0.12761	н	77
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28 0.2032 n 1.3 30 0.2328 C 1.3 31 0.6075 H 1.6 33 0.20255 H 1.7 33 0.20255 H 1.8 34 0.20616 H 2.21 33 0.2025 H 2.22 33 0.20616 H 2.21 33 0.2087 H 2.22 33 0.2087 H 2.22 33 0.2087 H 2.23 33 0.2087 H 2.22 44 0.60757 H 2.28 44 0.60357 H 2.24 44 0.6038 H 2.9 44 0.6037 C 2.44 45 0.20381 C 4.44 47 0.2328 H 4.44 46 0.2085 H 5.5 51 0.2128 H </td <td>L II</td> <td>27</td> <td>-0.61033</td> <td>н</td> <td>12</td>	L II	27	-0.61033	н	12
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31 -0.60753 H 13 32 0.20826 H 17 33 0.20256 H 18 333 0.20668 C 19 335 -0.6097 H 20 36 0.20616 H 21 337 0.199 H 22 38 0.2282 C 233 40 -0.60757 H 24 40 -0.60757 H 28 441 0.20826 H 26 442 0.20673 C 27 443 0.20257 H 28 444 -0.61035 H 29 445 0.20431 C 442 446 0.20327 H 442 446 0.203287 H 444 51 0.199 H 448 52 -0.31027 H 449 53 0.02038 H <td>н</td> <td>20</td> <td>0.2320</td> <td>C</td> <td>14</td>	н	20	0.2320	C	14
32 0.00326 H 17 33 0.20255 H 18 34 0.20668 C 19 35 0.6097 H 20 36 0.20616 H 21 37 0.199 H 22 33 0.2082 C 23 33 0.20673 C 27 41 0.20877 H 28 44 0.20873 C 27 443 0.20257 H 28 444 0.61035 H 29 443 0.20231 C 44 44 0.61035 H 29 444 0.61035 H 44 446 0.20382 H 44 45 0.20387 H 44 45 0.20387 H 44 56 0.2018 C 45 57 0.60596 C 50	C C	31	-0.60753	н	15
	н	31	0.20826	н	10
34 0.20668 C 19 35 -0.6097 H 20 36 0.20616 H 21 37 0.199 H 22 38 0.2282 C 233 40 -0.60757 H 24 40 -0.6073 C 277 43 0.2057 H 28 44 -0.61035 H 28 44 -0.61035 H 28 44 -0.61035 H 28 444 -0.60972 C 44 446 0.20327 H 44 447 0.23287 H 44 448 -0.60972 C 45 50 0.22814 H 47 49 0.20618 C 50 54 0.2085 H 51 55 0.2028 H 52 56 0.20128 H	н	33	0.20255	н	.18
33 -0.6097 H 20 336 0.20616 H 21 337 0.13064 H 223 339 -0.31064 H 224 40 -0.60757 H 225 41 0.20257 H 228 43 0.20257 H 228 44 -0.61035 H 29 445 0.20287 H 28 444 -0.61035 H 29 445 0.20287 H 243 446 0.20382 H 43 446 0.20382 H 443 446 0.20382 H 444 447 0.23287 H 444 448 -0.60972 C 445 550 0.2018 C 446 551 0.199 H 48 551 0.20178 H 55 560 0.20178	н	34	0.20668	С	19
36 0.20616 H 21 37 0.199 C 23 38 0.2282 C 23 40 -0.60757 H 26 41 0.20826 H 25 41 0.20257 H 26 42 0.20637 H 29 44 -0.61035 H 29 445 0.20382 H 44 -0.445 0.20382 H 44 -0.448 -0.02382 H 44 -0.448 -0.00382 H 44 -0.448 -0.0097 C 45 -0.20382 H 44 44 -0.20382 H 44 44 -0.20382 H 44 44 -0.20381 H 44 47 -50 0.20178 H 48 -51 0.199 H 48 -52 0.2065 <td< td=""><td>С</td><td>35</td><td>-0.6097</td><td>Н</td><td>20</td></td<>	С	35	-0.6097	Н	20
37 0.199 H 222 38 0.2282 C 233 39 -0.3106 H 224 40 -0.60757 H 255 41 0.20826 H 266 42 0.20673 C 277 43 0.20257 H 288 44 -0.61035 H 292 445 0.20431 C 442 446 0.20382 H 433 47 0.22387 H 443 446 0.60972 C 453 49 0.20618 C 466 50 0.2814 H 477 49 0.20618 C 505 51 0.1027 H 498 53 -0.60996 C 500 54 0.20178 H 513 55 0.20178 H 553 66 0.20239 C	Н	36	0.20616	н	21
38 0.2282 C 233 39 -0.31064 H 24 40 -0.60757 H 285 441 0.20826 H 265 442 0.20673 C 277 443 0.20257 H 288 444 -0.61035 H 299 445 0.20382 H 443 446 0.20382 H 443 447 0.23287 H 444 448 0.60018 C 446 50 0.22814 H 447 51 0.199 H 448 52 -0.31027 H 449 53 -0.60596 C 500 54 0.20885 H 51 55 0.20178 H 532 56 0.20178 H 55 59 0.2065 H 55 59 0.20267 <	Н	37	0.199	н	22
33 -0.31064 H 244 40 -0.60757 H 255 41 0.208673 C 277 43 0.20257 H 288 44 -0.61035 H 299 445 0.20832 H 242 446 0.20382 H 443 446 0.20382 H 444 448 -0.60972 C 445 50 0.20384 H 447 51 0.199 H 448 52 -0.31027 H 49 53 0.60596 C 50 54 0.20128 H 51 55 0.20128 H 53 56 0.20174	н	38	0.2282	С	23
40 -0.60757 H 225 41 0.20873 C 277 43 0.20673 C 277 43 0.20673 C 277 43 0.20431 C 442 44 -0.61035 H 299 445 0.20431 C 442 446 0.0382 H 433 47 0.2387 H 444 446 0.60972 C 455 49 0.20618 C 466 550 0.22814 H 477 49 0.20618 C 500 53 0.60996 C 500 54 0.20885 H 511 55 0.20178 H 532 55 0.20178 H 532 55 0.2029 H 57 61 0.61255 C 588 62 0.2037 H	С	39	-0.31064	н	24
41 0.20826 H 26 42 0.20673 C 27 43 0.20257 H 28 44 0.61035 H 29 44 0.20431 C 42 45 0.20431 C 42 445 0.20431 C 42 446 0.20382 H 43 47 0.23287 H 44 48 0.606972 C 45 49 0.20618 C 46 50 0.22814 H 47 51 0.199 H 48 53 0.60596 C 50 53 0.20128 H 51 54 0.20885 H 51 55 0.20178 H 53 56 0.20178 H 56 57 -6.6064 C 54 66 0.20137 H 6	С	40	-0.60757	н	25
42 0.20673 C 277 43 0.20257 H 288 44 -0.61035 H 29 45 0.20431 C 422 446 0.20382 H 433 47 0.23827 H 443 48 -0.60972 C 445 49 0.202814 H 447 50 0.22814 H 447 51 0.199 H 448 52 -0.31027 H 449 53 -0.60964 C 500 53 0.20178 H 533 55 0.20128 H 533 56 0.20178 H 533 57 -0.60964 C 544 58 0.20239 H 557 59 0.20147 H 566 61 -0.61255 C 588 62 0.20239 <	Н	41	0.20826	Н	26
43 0.20257 H 28 44 -0.61035 H 29 445 0.20321 C 42 446 0.20322 H 43 47 0.23287 H 443 447 0.23287 H 444 48 -0.60972 C 455 49 0.20618 C 466 50 0.22814 H 477 51 0.199 H 488 52 -0.31027 H 499 53 -0.60596 C 500 54 0.20885 H 51 55 0.20128 H 52 56 0.20178 H 53 57 -0.60964 C 54 58 0.2065 H 55 60 0.22399 C 599 63 0.2382 H 60 66 0.61247 C	н	42	0.20673	С	27
44 -0.61035 H 29 45 0.20431 C 442 46 0.20382 H 443 47 0.23287 H 443 47 0.23287 H 444 48 -0.60972 C 445 50 0.22814 H 447 51 0.199 H 488 52 -0.31027 H 449 53 -0.60596 C 500 54 0.2088 H 511 55 0.20128 H 521 56 0.20178 H 533 57 -0.60964 C 544 58 0.20247 H 555 59 0.20747 H 556 60 0.22399 H 577 61 -0.61255 C 588 62 0.20237 H 660 64 0.20137	н	43	0.20257	н	28
45 0.20431 C 442 46 0.20382 H 443 47 0.22877 H 444 48 0.60972 C 455 49 0.20618 C 466 50 0.22814 H 477 51 0.199 H 448 52 0.31027 H 499 53 -0.60596 C 500 54 0.20885 H 511 55 0.20178 H 533 56 0.20178 H 533 56 0.20178 H 533 57 -0.60964 C 544 58 0.2065 H 555 59 0.20747 H 566 60 0.23299 H 577 61 -0.61255 C 588 62 0.20237 H 661 64 0.20137 H<	С	44	-0.61035	Н	29
46 0.20382 H 43 47 0.23287 H 44 48 -0.60972 C 45 49 0.20518 C 46 50 0.22814 H 47 51 0.199 H 48 52 -0.31027 H 49 53 -0.60596 C 50 53 -0.60596 C 50 53 -0.60596 C 50 55 0.2018 H 51 55 0.20178 H 53 57 -0.60964 C 54 58 0.2065 H 55 59 0.20747 H 56 61 -0.61255 C 58 62 0.20237 H 61 65 -0.31066 H 62 66 -0.61247 C 63 66 0.20137 H <	н	45	0.20431	С	42
47 0.23287 H 444 48 -0.60972 C 445 49 0.20618 C 466 50 0.22814 H 477 51 0.199 H 488 52 -0.1027 H 499 53 0.2085 H 511 55 0.20128 H 521 55 0.20128 H 522 56 0.20178 H 533 57 -0.60964 C 544 58 0.2065 H 555 59 0.20747 H 566 60 0.22399 H 577 61 -0.61255 C 588 62 0.20239 C 599 63 0.23682 H 660 64 0.20137 H 611 65 0.31066 H 622 66 -0.61247 C<	Н	46	0.20382	н	43
48 -0.60972 C 455 49 0.20618 C 466 50 0.22814 H 477 51 0.199 H 488 52 -0.31027 H 499 53 -0.60985 C 500 54 0.20885 H 511 55 0.20128 H 522 56 0.20178 H 533 55 0.20285 H 533 56 0.20178 H 533 57 -0.60964 C 544 59 0.20747 H 555 60 0.22399 H 577 61 -0.61255 C 588 62 0.2029 C 599 63 0.2382 H 660 64 0.20137 H 641 65 -0.31066 H 622 66 0.61247	Н	47	0.23287	Н	44
49 0.20618 C 46 50 0.22814 H 47 51 0.199 H 48 52 -0.31027 H 49 53 -0.60596 C 500 54 0.2088 H 51 55 0.20128 H 52 56 0.20178 H 53 57 -0.60964 C 54 58 0.20747 H 55 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 H 60 63 0.2682 H 600 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 71 0.20651 H <t< td=""><td>С</td><td>48</td><td>-0.60972</td><td>С</td><td>45</td></t<>	С	48	-0.60972	С	45
S0 0.22814 H 47 51 0.199 H 448 52 0.31027 H 49 53 -0.60596 C 500 54 0.20885 H 51 55 0.20128 H 52 55 0.20128 H 53 55 0.20178 H 53 57 -0.60964 C 54 58 0.2065 H 55 59 0.20747 H 56 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 600 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 68 0.20146 H 65 70 0.20651 H <	Н	49	0.20618	С	46
51 0.199 H 48 52 -0.31027 H 49 53 -0.60596 C 50 54 0.20885 H 51 55 0.20128 H 52 56 0.20178 H 53 57 -0.60964 C 54 58 0.2065 H 55 59 0.20747 H 56 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 69 0.2367 H 66 70 -0.6096 C 677 71 0.20651 H <td< td=""><td>н</td><td>50</td><td>0.22814</td><td>H</td><td>47</td></td<>	н	50	0.22814	H	47
52 -U.3102/ 0.3102/ H 449 53 -0.60596 C 50 54 0.20885 H 51 55 0.20128 H 51 55 0.20178 H 53 57 -0.60964 C 54 58 0.2065 H 55 59 0.20747 H 56 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 66 64 0.20137 H 61 65 -0.61247 C 63 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 70 -0.6096 C 677 71 0.20651 H 68 72 0.224 H	п	51	0.199	н	48
	c	52	-0.31027	H C	49
ST 0.20000 In 31 55 0.20128 H 52 56 0.20178 H 53 57 -0.60964 C 54 58 0.20239 H 55 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 66 63 0.23682 H 66 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 70 0.6096 C 67 71 0.20237 H 68 72 0.2024 H 69 72 0.2024 H 69 72 0.2024 H 6	н	53	-U.60596	ц	50 E1
10 10 <th10< th=""> 10 10 10<!--</td--><td>н</td><td>55</td><td>0.20128</td><td>н</td><td>51</td></th10<>	н	55	0.20128	н	51
57 -0.60964 C 53 58 0.2065 H 55 60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 66 -0.61247 C 63 67 0.20237 H 64 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 70 -0.6096 C 677 71 0.20651 H 68 72 0.224 H 69 73 0.20747 H 70 76 0.20179 H 73 77 0.20131 H <t< td=""><td>н</td><td>56</td><td>0.20178</td><td>н</td><td>53</td></t<>	н	56	0.20178	н	53
58 0.2065 H 55 59 0.20747 H 56 60 0.22399 H 57 61 -0.61255 C 58 62 0.2039 C 59 63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 66 -0.61247 C 63 66 -0.61247 C 63 66 0.20237 H 664 67 0.20237 H 664 66 -0.61247 C 633 67 0.20267 H 666 70 -0.6096 C 677 71 0.20651 H 68 72 0.2224 H 69 73 0.20747 H 70 75 0.20888 H	С	57	-0.60964	C	54
S9 0.20747 H S6 60 0.22399 H S7 61 -0.61255 C S8 62 0.20239 C S9 63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 69 0.2367 H 666 70 -0.6096 C 67 71 0.2051 H 68 72 0.224 H 69 73 0.20747 H 70 74 -0.60601 C 71 75 0.2088 H 72 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum <td< td=""><td>н</td><td>58</td><td>0.2065</td><td>Н</td><td>55</td></td<>	н	58	0.2065	Н	55
60 0.22399 H 57 61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 0.61247 C 63 67 0.20237 H 64 68 0.20146 H 655 69 0.2367 H 64 68 0.20146 H 655 70 -0.6096 C 67 71 0.20251 H 68 72 0.224 H 69 73 0.20747 H 70 75 0.2088 H 72 76 0.20179 H 73 77 0.20131 H 74 76 0.20179 H 73 77 0.20131 H 74	Н	59	0.20747	Н	56
61 -0.61255 C 58 62 0.20239 C 59 63 0.23682 H 600 64 0.2017 H 61 65 -0.31066 H 62 66 -0.61247 C 63 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 655 69 0.2367 H 666 70 -0.6096 C 677 71 0.20651 H 688 72 0.224 H 69 73 0.20747 H 700 74 -0.60601 C 711 76 0.20179 H 733 77 0.20131 H 74 76 0.20179 H 733 77 0.20131 H 74 30 117158 Sum	Н	60	0.22399	Н	57
62 0.20239 C 99 63 0.2362 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 62 69 0.2367 H 66 70 -0.6096 C 67 71 0.20651 H 68 72 0.224 H 69 73 0.20747 H 70 73 0.20747 H 70 76 0.20179 H 73 77 0.20131 H 74 5um 1.17158 Sum 30 77 0.20131 H 74 Sum 1.17158 Sum 30 4 -0.64702 N 30 13 -0.20176 C <	С	61	-0.61255	С	58
63 0.23682 H 60 64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.2046 H 65 69 0.20237 H 66 70 0.20237 H 66 69 0.2037 H 66 70 -0.6096 C 67 70 0.20651 H 68 71 0.20651 H 68 77 0.2024 H 69 73 0.20747 H 70 74 -0.60601 C 71 75 0.2088 H 72 76 0.20179 H 73 9 -0.64702 N 30 117158 Sum 4 -0.64702 N 30 13 -0	Н	62	0.20239	С	59
64 0.20137 H 61 65 -0.31066 H 62 66 -0.61247 C 63 67 0.20237 H 64 68 0.20146 H 65 69 0.2367 H 66 70 -0.6096 C 677 71 0.20651 H 68 72 0.224 H 699 73 0.20747 H 70 74 -0.60601 C 71 75 0.2088 H 72 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 50 4 -0.64716 N 30 3 -0.20131 C 33 112 0.14538 C 32 3 -0.64702 N 30 3 0.4943 B <td< td=""><td>H</td><td>63</td><td>0.23682</td><td>н</td><td>60</td></td<>	H	63	0.23682	н	60
bb -0.31066 H 662 66 -0.61247 C 633 67 0.20237 H 664 68 0.20146 H 655 69 0.2367 H 666 70 -0.6096 C 677 71 0.20551 H 688 72 0.224 H 669 73 0.20747 H 700 73 0.20747 H 700 75 0.2088 H 720 75 0.2088 H 723 76 0.20179 H 733 77 0.20131 H 744 Sum 1.17158 Sum 10.04716 8 0.4943 B 331 12 0.14538 C 322 13 -0.26013 C 344 0.20716 C 344 14 0.20716 C <t3< td=""><td>н</td><td>64</td><td>0.20137</td><td>Н</td><td>61</td></t3<>	н	64	0.20137	Н	61
bb -U.0.1247 C 63 67 0.20237 H 64 68 0.2014 H 65 69 0.2367 H 66 70 -0.6096 C 67 71 0.20651 H 68 72 0.224 H 69 73 0.20747 H 69 73 0.20747 H 70 73 0.20747 H 70 74 -0.60601 C 71 75 0.20179 H 73 76 0.20179 H 73 77 0.20131 H 74 5 -0.64716 N 4 Sum 1.17158 Sum 4 18 0.4943 B 31 13 -0.26013 C 33 13 -0.26013 C 34 14 0.20716 C 3	C	65	-0.31066	H	62
or/ 0.2023/ H 64 68 0.20146 H 655 69 0.2367 H 666 70 -0.6096 C 677 71 0.20651 H 668 72 0.224 H 669 73 0.20747 H 700 75 0.20179 H 733 77 0.20131 H 774 Sum 1.17158 Sum 900 5 -0.64702 N 300 112 0.14538 C 322 113 -0.26013 C 333 14 0.20716 C 344 15 0.14542 H 337 116 -0.22648 <	с u	66	-U.01247		63
GO 0.20440 P GS 69 0.2367 H 666 70 -0.6096 C 677 71 0.20651 H 689 72 0.2041 H 689 73 0.20747 H 699 73 0.20747 H 700 74 -0.60601 C 711 75 0.2088 H 712 76 0.20179 H 733 77 0.20131 H 744 78 0.20131 H 744 78 0.20131 H 74 79 0.20131 H 74 70 0.20131 H 74 5 -0.64702 N 300 18 0.4943 B 313 12 0.14538 C 332 14 0.20716 C 334 15 0.14542 H	а	6/	0.2023/	п ⊔	64
00 0.200 n 000 70 0.2009 C 677 71 0.20651 H 688 72 0.224 H 699 73 0.20747 H 700 74 0.60601 C 71 75 0.20888 H 722 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64702 N 30 118 0.4943 B 31 12 0.14538 C 33 13 -0.26013 C 333 14 0.20716 C 344 15 0.14542 H 355 16 -0.22648 C 36 17 0.20471 H 39 20 0.20472 H 39 21 0.2601 C 38 </td <td>н</td> <td>68 20</td> <td>0.20146</td> <td>п ц</td> <td>65</td>	н	68 20	0.20146	п ц	65
71 0.2051 H 68 71 0.2051 H 68 72 0.224 H 69 73 0.20747 H 70 74 0.60601 C 71 75 0.2088 H 72 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64716 N 4 0.64702 N 300 18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 34 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21<	C	09 70	-0.230/	C	67
72 0.224 H 66 73 0.20747 H 66 73 0.20747 H 70 74 -0.60601 C 71 75 0.2088 H 72 76 0.20179 H 73 77 0.20131 H 73 77 0.20131 H 73 9 0.40416 N 4 5 -0.64716 N 4 4 -0.60176 N 30 118 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 39 20 0.20472 H 39 21 -0.2601 C 40 <td>н</td> <td>70</td> <td>0.20651</td> <td>н</td> <td>68</td>	н	70	0.20651	н	68
73 0.20747 H 70 73 0.20747 H 70 74 -0.60601 C 71 75 0.20888 H 72 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64716 N 44 5 -0.64702 N 300 18 0.4943 B 31 12 0.14538 C 332 13 -0.26013 C 333 14 0.20716 C 34 15 0.14542 H 355 16 -0.22648 C 36 17 0.20471 H 37 19 -0.2647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 31 <	н	72	0.274	н	69
74 -0.66601 C 71 75 0.20888 H 72 76 0.20179 H 73 77 0.20131 H 74 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64716 N 44 5 -0.64702 N 300 18 0.4943 B 31 12 0.14538 C 332 14 0.20716 C 334 15 0.14542 H 355 16 -0.22648 C 366 17 0.20471 H 377 19 -0.22647 C 388 20 0.20472 H 399 21 -0.2601 C 40 22 0.20715 H 41	н	73	0.20747	н	70
75 0.20888 H 72 76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64702 N 30 18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 355 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 5um -0.6552 Sum 5um	С	74	-0.60601	C	71
76 0.20179 H 73 77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64716 N 44 5 -0.64702 N 300 18 0.4943 B 311 12 0.14538 C 322 13 -0.26013 C 334 14 0.20716 C 344 15 0.14542 H 335 16 -0.22648 C 366 17 0.20471 H 37 9 -0.22647 C 38 20 0.20472 H 39 21 -0.26017 C 44 20 0.20472 H 39 21 -0.26017 C 44 39 -0.65852 Sum	н	75	0.20888	н	72
77 0.20131 H 74 Sum 1.17158 Sum 4 -0.64716 N 44 5 -0.64702 N 300 18 0.4943 B 311 12 0.14538 C 322 13 -0.26013 C 333 14 0.20716 C 344 15 0.14542 H 335 16 -0.22648 C 366 17 0.20471 H 337 19 -0.22647 C 388 20 0.20472 H 339 21 -0.26015 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	Н	76	0.20179	Н	73
Sum 1.17158 Sum 4 -0.64716 N 4 5 -0.64702 N 30 18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.26647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 5um -0.65852 Sum 5um	н	77	0.20131	Н	74
4 -0.64716 N 4 -0.64702 N 30 18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 333 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.26647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum 500		Sum	1.17158		Sum
5 -0.64702 N 30 18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 333 14 0.20716 C 334 15 0.14542 H 355 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	Ν	4	-0.64716	N	4
18 0.4943 B 31 12 0.14538 C 32 13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	Ν	5	-0.64702	N	30
12 0.14538 C 32 13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	В	18	0.4943	В	31
13 -0.26013 C 33 14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	С	12	0.14538	С	32
14 0.20716 C 34 15 0.14542 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	C	13	-0.26013	С	33
15 0.14942 H 35 16 -0.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	н	14	0.20716	C	34
16 -U.22648 C 36 17 0.20471 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum Sum	C	15	0.14542	H	35
17 0.2047 H 37 19 -0.22647 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.2015 H 41 Sum -0.65852 Sum Sum	L L	16	-0.22648	C	36
13 -0.22047 C 38 20 0.20472 H 39 21 -0.2601 C 40 22 0.20715 H 41 Sum -0.65852 Sum	ri C	17	0.20471	H	37
20 0.201/2 n 39 21 -0.2601 C 40 22 -0.20715 H 41 Sum -0.65852 Sum Sum		19	-0.22047 0 20/172	н	38
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