## **Electronic Supplementary Information**

on

## Enhancing NIR-to-visible photon upconversion in cast solid by introducing bulky substituents in rubrene and by suppressing back energy transfer

by

Akane Sawa,<sup>a,b</sup> Shota Shimada,<sup>a,b</sup> Neeti Tripathi,<sup>a</sup> Claire Heck,<sup>a</sup> Hiroaki Tachibana,<sup>c</sup>

Emiko Koyama, <sup>c</sup> Toshiko Mizokuro, <sup>c</sup> Yasukazu Hirao, <sup>d</sup> Takashi Kubo, <sup>d</sup> Naoto Tamai, <sup>b</sup>

Daiki Kuzuhara,<sup>e</sup> Hiroko Yamada, <sup>f</sup> and Kenji Kamada<sup>a,b,\*</sup>

<sup>a</sup>Nanomaterials Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan

<sup>b</sup>Department of Chemistry, Graduate School of Science and Technology, Kwansei Gakuin University, Sanda 669-1337, Japan

<sup>c</sup>Research Institute for Advanced Electronics and Photonics, National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

<sup>d</sup>Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka, 560-0043, Japan

<sup>e</sup>Department of Physical Science and Materials Engineering, Iwate University, Morioka, Iwate 020-8551, Japan

<sup>f</sup>Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST), Ikoma, Nara 630-0192, Japan

## Contents (in appearance order)

Fig. S1. <sup>1</sup>H-NMR spectrum of **DMeORb**. Fig. S2. <sup>13</sup>C-NMR spectrum of **DMeORb**. Fig. S3. <sup>1</sup>H-NMR spectrum of **DOcORb**. Fig. S4. <sup>13</sup>C-NMR spectrum of **DOcORb**. Fig. S5. X-ray crystal structure of **TBRb** and **DOcORb**. Table S1. Crystallographic data for TBRb and DOcORb. Fig. S6. Example of absorption spectrum of cast film (PdTPTAP:TBRb) measured by using microspectroscopic setup. Fig. S7. Spectra of laser scattering and UC emission by nanosecond excitation. Fig. S8. Polarization microscopic images of the mixed cast films. Fig. S9. Microscopic images of the pristine cast film of **TBRb**. Fig. S10. Bidirectional excitation intensity dependence of the UC emission intensity. Fig. S11. The excitation intensity dependence of UC emission efficiency. Fig. S12. Spectral overlap between the fluorescence spectrum of emitters and the absorption spectrum of sensitizer. Fig. S13. Prompt fluorescence decay of the pristine TBRb cast solids. Fig. S14. Sensitizer concentration dependence of  $I_{\rm th}$  for the mixed cast solids. Fig. S15. UC emission time profiles in short- and long-time scale plotted to the same vertical scale. Fig. S16. Nanosecond emission time profile of the mixed cast films with different concentration ratios excited by nanosecond laser pulses. Fig. S17. Nanosecond emission time profile of the pristine emitter films excited by femtosecond laser pulses. Fig. S18. Nanosecond emission time profile of the TBRb cast films with and without the sensitizer excited by nanosecond laser pulses. Fig. S19. Microsecond-scale emission time profiles of the mixed cast films with different concentration ratios excited by nanosecond laser pulses. Table S2. Best fit parameters to the microsecond-scale emission time profile presented in Fig. S14 by eq. 3. Fig. S20. Plot of the TTA quantum yield calculated by  $\eta_{UC}$  /  $\Phi_{FL}$  and  $\eta_{\rm UC} / (\Phi_{\rm FL} \Phi_{\rm TET}).$ Table S3. Optimized geometry of the singlet ground state of rubrene (**Rb**). Table S4. Optimized geometry of the triplet ground state of rubrene (**Rb**).

- Table S5.Optimized geometry of the singlet ground state of TBRb.
- Table S6.Optimized geometry of the triplet ground state of TBRb.
- Table S7.Optimized geometry of the singlet ground state of **DMeORb**.
- Table S8.Optimized geometry of the triplet ground state of **DMeORb**.
- Table S9.Optimized geometry of the singlet ground state of **DOcORb**.
- Table S10.Optimized geometry of the triplet ground state of **DOcORb**.















**Fig. S5.** X-ray crystal structure of **TBRb** and **DOcORb** (only these two of the three derivatives could be defined successfully). a-, b-, and c-axis are shown in red, green, and blue, respectively (in the top row, c-axis is normal to the sheet).

DOcORb

Compound	TBRb	DOcORb
empirical formula	$C_{58}H_{60}$	C58H59O2
formula weight	757.06	788.05
<i>T</i> (K)	293(2)	346.15
crystal system	triclinic	monoclinic
space group	P 1	P 1 21/n 1
<i>a</i> (Å)	6.7599(3)	12.0181(5)
<i>b</i> (Å)	12.3329(5)	27.3671(10)
<i>c</i> (Å)	14.0691(4)	14.8672(6)
$\alpha$ (degree)	92.553(3)	90
$\beta$ (degree)	99.746(3)	108.077(4)
γ (degree)	104.374(3)	90
cell volume (Å <sup>3</sup> )	1115.20(7)	4648.5(3)
Ζ	1	4
density (g cm $^{-3}$ )	1.127	1.126

## **Table S1.** Crystallographic data for **TBRb** and **DOcORb**.



Fig. S6. Example of absorption spectrum of PdTPTAP:TBRb cast film (concentration ratio [PdTPTAP]:[TBRb] = 1:20000) after baseline correction measured by using the microspectroscopic system (red line) together with the solution spectrum of PdTPTAP in tetrahydrofuran (blue line). The solution spectrum was scaled to match the film spectrum.



**Fig. S7.** (a) Spectrum of laser scattering (red) was totally blocked by inserting a 700-nm short-pass filter in the detection path (green), and further added two excitation-cut filters (blue). (b) Emission spectrum of **PdTPTAP:TBRb** film ([sensitizer]:[emitter]=1:2000) through the 700-nm short-pass filter (green) and further added the two excitation-cut filters (blue). The 700-nm short-pass filter (Thorlabs FESH0700) was O.D. >5 at 800 nm and the excitation cut filter (Hoya E-CM500S) was O.D. 3 at 800 nm for a single piece. All data was excited by 800-nm nanosecond laser pulses (10 ns, 1 kHz, 22 kW cm<sup>-2</sup> at the sample position) and detected by the same detection optics except for the filter combinations. A SMA-connected fiber spectrometer (OceanOptics USB2000) was used instead of the SMA-connecter terminated optical fiber from the detection optics. Spectral correction for the spectrometer was not applied for these data.



**Fig. S8.** Parallel polarization (left column) and crossed Nicole (right column) microscopic transmission images of the mixed cast films of the rubrene derivatives: (a) **TBRb**, (b)**DMeORb**, and (c) **DOcORb** with the molar ratio of [sensitizer] : [emitter]=1 : 2000. The bars indicate 100 μm.



**Fig. S9.** Microscopic transmission images of the cast films of pristine **TBRb**, at different sample positions ((a) and (b)). The bars indicate 100 μm.



**Fig. S10.** Bidirectional excitation intensity dependence of the upconverted emission of the mixed cast solid films of (a) **PdTPTAP:TBRb**, (b) **PdTPTAP:DMeORb**, and (c) **PdTPTAP: DOcORb**, excited at 785 nm by cw irradiation. The concentration ratio was [**PdTPTAP**]:[**emitter**] = 1:2000 for all. The excitation intensity increased and then decreased during the measurement (*i.e.*, round trip).



Fig. S11. The excitation intensity dependence of upconversion quantum efficiency  $\eta_{UC}$  of the mixed cast solid films of (a) PdTPTAP:TBRb, (b) PdTPTAP:DMeORb, and (c) PdTPTAP: DOcORb, excited at 785 nm by cw irradiation. The concentration ratio was [PdTPTAP]:[emitter] = 1:2000 for all. These data were obtained after processing the data in Fig. 4. The solid curves are the curve fits with the theoretical expression,  $\eta_{UC} = a\left(1 + \frac{1-\sqrt{1+2bx}}{bx}\right)$  where x and b are the same as in eq. 1 in the main text but  $a = \eta_{UC}^{\infty}$ , the maximum UC efficiency for the strong excitation limit [from Y. Murakami, K. Kamada, *Phys. Chem. Chem. Phys.* 2021, 23, 18268].



Fig. S12. Overlap of the area-normalized fluorescence spectrum (black curve) of emitter: (a) TBRb, (b)DMeORb, and (c) **DOcORb** and the absorption spectrum of sesitizer (PdTPTAP in toluene, red curve). The calculated value of overlap integral *J* is shown in each panel.



**Fig. S13.** Prompt fluorescence decay curves of the pristine (pure) cast solids of **TBRb** (symbol) excited at  $520\pm10$  nm with the double-exponential fit (solid line).



Fig. S14. Sensitizer concentration dependence of  $I_{th}$  for the mixed cast solids with the rubrene derivatives: PdTPTAP:TBRb (red circle), PdTPTAP:DMeORb (green square), and PdTPTAP:DOcORb (blue diamond).



**Fig. S15.** Upconversion emission time profile of the mixed films (solid line) of (a) **PdTPTAP:TBRb**, (b) **PdTPTAP:DMeORb**, and (c) **PdTPTAP:DOcORb** recorded in short (-0.1 to 0.4  $\mu$ s, linear) and long (0.4 to 100  $\mu$ s, logarithmic) time scales plotted to the same vertical axis. The data are normalized at 0  $\mu$ s for the short-scale data. Magnitude of the long-scale data was scaled so that they matched to the short-scale data at the overlap time (0.4  $\mu$ s). The data of each film was vertically shifted for visibility. The dotted lines are also the long-scale data but plotted with vertical magnification with the shown factors. The concentration ratio of the samples was [sensitizer]:[emitter] = 1:2000. The samples were excited by nanosecond pulses at 800 nm (10 ns, 22 kW cm<sup>-2</sup>, at 1 kHz repetition).



**Fig. S16.** Nanosecond-scale time profile of upconversion emission of the mixed films of (a),(d) **PdTPTAP:TBRb**, (b),(d) **PdTPTAP:DMeORb**, and (c),(f) **PdTPTAP:DOcORb** with different concentration ratios of the sensitizer and the corresponding emitter as shown in each panel. The samples were excited by nanosecond pulses at 800 nm (10 ns, at 1 kHz repetition) with 22 kW cm<sup>-2</sup> ((a)-(c)) and 6.5 kW cm<sup>-2</sup> ((d)–(f)). Emission at the wavelengths shorter than 700 nm was detected through 700-nm short pass and two excitation cut filters.



**Fig. S17.** Time profile of the prompt fluorescence (red solid curve) of the pristine films (no sensitizer) of (a) **TBRb**, (b) **DMeORb**, and (c) **DOcORb** by two-photon excitation with femtosecond laser pulses (800 nm, 120 fs, 4.2 GW cm<sup>-2</sup>). The results of convolution (green dash-and-dotted curve) of the material response of the exponential decay time constant ( $\tau =$  (a) 4 ns, (b) 4 ns, (c) 5 ns) with the instrumental response function (black dotted curve) are also presented. The same detection setup was used as for the nanosecond excitation measurements as in Figs. S15 and S16, S18. Emission at the wavelengths shorter than 700 nm was detected.



**Fig. S18.** Emission time profile of **TBRb** cast films without (pristine, blue dashed curve) and with **PdTPTAP** ([sensitizer]:[emitter]=1:1000, red solid curve), both excited by nanosecond laser pulses (10 ns, 1 kHz, 6.5 kW cm<sup>-2</sup>). Emission at the wavelengths shorter than 700 nm was detected.



**Fig. S19.** Semi-log plot of the microsecond-scale time profiles of UC emission of the mixed films of (a) **PdTPTAP:TBRb**, (b) **PdTPTAP:DMeORb**, and (c) **PdTPTAP:DOcORb** with various concentration ratios (from bottom to top, [sensitizer]:[emitter] = 1:500, 1:2000, 1:2000, 1:2000) excited by nanosecond laser pulses (10 ns, 22 kW cm<sup>-2</sup>). One division of the vertical scale is ten times. Each data was shifted vertically by one division for readability.

Emitter	Α	В	$ au_R$ / $\mu s$	$ au_D$ / $\mu s$	f	$ au_{ ext{TET}}^{ ext{slow}}$	$ au_{ ext{TET}}^{ ext{fast}}$	$\langle  au_{\mathrm{TET}}  angle$	Фтет
[S]:[E]						/ μs	/ <b>ns</b>	/ µs	
TBRb									
1:500	72%	28%	6.6	92.6	0	6.2	40	1.7	90%
1:2000	74%	26%	10.9	90.7	0	9.7	40	2.5	85%
1:5000	78%	22%	17.6	89.5	0	14.7	20	3.2	80%
1:10000	81%	19%	21.6	93.2	0	17.6	40	3.3	80%
1:20000	100%	0%		109	0	109	40	0.0	100%
DMeORb									
1:500	64%	36%	0.8	39.4	0.629	0.8	40	0.3	98%
1:2000	62%	38%	1.1	77.3	0.490	1.1	40	0.4	98%
1:5000	65%	35%	1.4	106.8	0.317	1.4	20	0.5	97%
1:10000	72%	28%	2.0	139.6	0.158	2.0	40	0.5	97%
1:20000	78%	22%	0.0	99.7	0.136	2.0	40	0.4	97%
DOeORb									
1:500	64%	36%	3.2	110.9	0.425	3.1	40	1.1	93%
1:2000	62%	38%	3.8	154.3	0.000	3.7	40	1.4	91%
1:5000	64%	36%	4.7	170.3	0.000	4.6	20	1.7	90%
1:10000	68%	32%	5.3	195.8	0.000	5.2	40	1.6	90%
1:20000	75%	25%	0.0	193.6	0.000	7.4	40	1.8	89%

**Table S2.** Best fit parameters to the microsecond-scale emission time profile presented in Fig.S14 by eq. 3.



Fig. S20. Plot of the TTA quantum yield calculated by  $\eta_{UC} / \Phi_{FL}$  and  $\eta_{UC} / (\Phi_{FL} \Phi_{TET})$  of the mixed films of (a) PdTPTAP:TBRb, (b) PdTPTAP:DMeORb, and (c) PdTPTAP:DOcORb with various concentration ratios. The data from Fig. 6 and Table S2 are used.

Table	<b>Table S3.</b> Optimized geometry of the singlet ground state of rubrene ( <b>Rb</b> ) at B3LYP/6-31G(d).							
С	0.6	9913	-2.44867	0.19311	C	1.40820	-1.23468	0.25030
С	1.3	2011	-3.71539	0.47188	С	2.82223	-1.25633	0.74295
С	0.6	6474	-4.89520	0.25660	С	3.09634	-0.75864	2.02705
С	-0.6	6477	-4.89520	-0.25661	С	4.38078	-0.83328	2.56571
С	-1.3	2012	-3.71538	-0.47190	С	5.41744	-1.40671	1.82786
С	-0.6	9912	-2.44867	-0.19315	С	5.15781	-1.90836	0.55088
С	-1.4	0818	-1.23466	-0.25033	C	3.87124	-1.84006	0.01697
С	-2.8	2224	-1.25627	-0.74291	Н	2.33716	-3.72565	0.84405
С	-3.0	9640	-0.75860	-2.02700	Н	1.16230	-5.83867	0.46502
С	-4.3	8087	-0.83320	-2.56559	Н	-1.16235	-5.83866	-0.46502
С	-5.4	1752	-1.40654	-1.82765	Н	-2.33717	-3.72563	-0.84408
C	-5.1	5784	-1.90816	-0.55067	Н	-2.28978	-0.31818	-2.60687
C	-3.8	7123	-1.83991	-0.01684	Н	-4.56992	-0.44745	-3.56425
C	-0.7	2784	-0.00000	-0.00001	Н	-6.41958	-1.46448	-2.24454
C	0.7	2789	-0.00001	-0.00003	Н	-5.95894	-2.35400	0.03314
C	1.4	0821	1.23466	-0.25033	Н	-3.67643	-2.22822	0.97845
C	2.8	2225	1.25630	-0.74297	Н	2.28966	0.31861	-2.60710
С	3.0	9632	0.75889	-2.02718	Н	4.56974	0.44800	-3.56458
C	4.3	8077	0.83355	-2.56582	Н	6.41951	1.46469	-2.24477
С	5.4	1747	1.40671	-1.82783	Н	5.95903	2.35377	0.03312
С	5.1	5789	1.90807	-0.55074	Н	3.67657	2.22788	0.97853
С	3.8	7130	1.83976	-0.01684	Н	2.33718	3.72565	-0.84406
С	0.6	9915	2.44867	-0.19311	Н	1.16236	5.83866	-0.46498
С	1.3	2014	3.71539	-0.47187	Н	-1.16229	5.83866	0.46509
С	0.6	6478	4.89520	-0.25657	Н	-2.33713	3.72564	0.84411
С	-0.6	6472	4.89520	0.25665	Н	-2.28972	0.31839	2.60696
C	-1.3	2008	3.71538	0.47193	Н	-4.56985	0.44770	3.56434
C	-0.6	9910	2.44867	0.19314	Н	-6.41955	1.46452	2.24453
C	-1.4	0816	1.23466	0.25031	Н	-5.95896	2.35382	-0.03325
C	-2.8	2222	1.25628	0.74289	Н	-3.67646	2.22801	-0.97856
C	-3.0	9636	0.75874	2.02705	Н	2.28971	-0.31815	2.60685
C	-4.3	8083	0.83335	2.56563	Н	4.56978	-0.44751	3.56437
C	-5.4	1750	1.40658	1.82764	Н	6.41947	-1.46468	2.24481
C	-5.1	5785	1.90807	0.55061	Н	5.95892	-2.35427	-0.03286
C	-3.8	7124	1.83981	0.01678	Н	3.67647	-2.22840	-0.97831

Table	e <b>S4</b> .	Optimi	zed geometry of	of the triplet grou	und sta	te of rubrene (	<b>Rb</b> ) at B3LYP	/6-31G(d).
С	0.6	59065	2.48079	-0.19286	С	1.40527	1.22204	-0.27561
С	1.3	31695	3.71870	-0.44357	С	2.79788	1.22675	-0.81197
С	0.6	55658	4.92762	-0.23545	С	3.04421	0.64586	-2.06765
С	-0.6	55663	4.92762	0.23542	С	4.31503	0.68586	-2.64060
С	-1.3	31699	3.71870	0.44356	С	5.36889	1.30516	-1.96692
С	-0.6	59068	2.48079	0.19287	С	5.13960	1.88592	-0.71784
С	-1.4	10529	1.22203	0.27564	С	3.86667	1.85338	-0.15001
С	-2.7	79789	1.22675	0.81202	Н	2.34223	3.73163	-0.79259
С	-3.0	04420	0.64593	2.06774	Н	1.17321	5.86350	-0.43033
С	-4.3	31501	0.68596	2.64070	Н	-1.17327	5.86350	0.43028
С	-5.3	36889	1.30521	1.96700	Н	-2.34227	3.73162	0.79257
С	-5.1	L3962	1.88591	0.71790	Н	-2.22515	0.16730	2.59747
С	-3.8	36669	1.85335	0.15005	Н	-4.48004	0.23625	3.61662
С	-0.7	73480	-0.00000	0.00002	Н	-6.36046	1.33572	2.41089
С	0.7	73478	0.00000	0.00002	Н	-5.95498	2.36402	0.18118
С	1.4	10528	-1.22203	0.27562	Н	-3.69957	2.29869	-0.82617
С	2.7	79789	-1.22674	0.81198	Н	2.22519	-0.16724	2.59741
С	3.0	04423	-0.64588	2.06767	Н	4.48010	-0.23613	3.61651
С	4.3	31506	-0.68588	2.64061	Н	6.36050	-1.33563	2.41076
С	5.3	36892	-1.30514	1.96690	Н	5.95498	-2.36399	0.18109
С	5.1	13962	-1.88588	0.71781	Н	3.69954	-2.29870	-0.82621
С	3.8	36668	-1.85334	0.14999	Н	2.34226	-3.73164	0.79256
С	0.6	59067	-2.48079	0.19286	Н	1.17324	-5.86351	0.43028
С	1.3	31697	-3.71870	0.44355	Н	-1.17324	-5.86350	-0.43032
С	0.6	55660	-4.92763	0.23541	Н	-2.34226	-3.73162	-0.79257
С	-0.6	55660	-4.92762	-0.23545	Н	-2.22520	-0.16704	-2.59730
С	-1.3	31697	-3.71870	-0.44357	Н	-4.48008	-0.23597	-3.61646
С	-0.6	59066	-2.48079	-0.19287	Н	-6.36044	-1.33571	-2.41088
C	-1.4	10528	-1.22204	-0.27561	Н	-5.95491	-2.36431	-0.18133
С	-2.7	79788	-1.22677	-0.81200	Н	-3.69950	-2.29898	0.82604
C	-3.0	)4422	-0.64579	-2.06764	Н	2.22518	0.16719	-2.59737
C	-4.3	31503	-0.68581	-2.64061	Н	4.48008	0.23609	-3.61649
C	-5.3	36887	-1.30521	-1.96700	Н	6.36047	1.33564	-2.41079
C	-5.1	L3957	-1.88608	-0.71797	Н	5.95495	2.36406	-0.18114
C	-3.8	36665	-1.85352	-0.15011	Н	3.69953	2.29876	0.82618

Table	e <b>S5.</b> Optimiz	ed geometry o	of the singlet gro	ound sta	ate of <b>TBRb</b> at	B3LYP/6-310	G(d).
С	-0.64194	-2.46546	-0.51787	Н	2.24813	3.74543	-1.18263
С	-1.23493	-3.74435	-0.80720	Н	2.30387	0.37249	-2.91699
С	-0.57995	-4.93290	-0.61011	Н	4.58573	0.56631	-3.86017
С	0.75639	-4.87518	-0.08715	Н	6.39692	1.63793	-2.53023
С	1.39020	-3.68784	0.13605	Н	5.89600	2.51463	-0.25532
С	0.75252	-2.42931	-0.13416	Н	3.61290	2.31794	0.67716
С	1.43560	-1.20211	-0.06918	Н	-2.30383	-0.37247	-2.91701
С	2.84710	-1.19714	0.42732	Н	-4.58567	-0.56626	-3.86025
С	3.11881	-0.69147	1.70865	Н	-6.39691	-1.63787	-2.53035
С	4.40124	-0.74467	2.24622	Н	-5.89605	-2.51457	-0.25543
С	5.47762	-1.30135	1.53485	Н	-3.61297	-2.31791	0.67711
С	5.19834	-1.80896	0.25884	С	-2.63537	-6.18154	-1.47928
С	3.91188	-1.76469	-0.28109	С	-1.28066	-7.13091	0.39665
С	0.72780	0.01796	-0.31778	С	-0.33879	-7.05281	-1.94415
С	-0.72782	-0.01796	-0.31777	Н	-1.90481	-6.62913	1.14488
С	-1.43563	1.20212	-0.06919	Н	-0.29073	-7.28739	0.83815
С	-2.84712	1.19713	0.42734	Н	-1.71535	-8.11821	0.19742
С	-3.11877	0.69163	1.70875	Н	-3.31519	-5.68332	-0.77921
С	-4.40120	0.74484	2.24634	Н	-3.03883	-7.18088	-1.67895
С	-5.47763	1.30132	1.53490	Н	-2.64963	-5.62311	-2.42189
С	-5.19841	1.80874	0.25880	С	2.63540	6.18153	-1.47924
С	-3.91195	1.76447	-0.28114	С	1.28069	7.13089	0.39670
C	-0.75255	2.42932	-0.13418	С	0.33882	7.05283	-1.94410
C	-1.39020	3.68785	0.13605	Н	0.28312	6.49447	-2.88553
C	-0.75638	4.87519	-0.08714	Н	0.76748	8.03961	-2.15842
C	0.57996	4.93290	-0.61009	Н	-0.68450	7.20604	-1.58550
C	1.23492	3.74435	-0.80720	Н	1.90484	6.62910	1.14492
С	0.64192	2.46546	-0.51788	Н	0.29077	7.28738	0.83819
C	1.38042	1.26813	-0.56636	Н	1.71540	8.11819	0.19747
C	2.79738	1.32331	-1.04951	Н	3.31521	5.68329	-0.77918
C	3.09421	0.83516	-2.33207	Н	3.03887	7.18086	-1.67890
C	4.37959	0.94644	-2.86271	H	2.64965	5.62311	-2.42186
C	5.39477	1.54954	-2.11882	Н	-0.28308	-6.49444	-2.88556
C	5.11263	2.04257	-0.84301	H	-0.76743	-8.03959	-2.15848
C	3.82548	1.93524	-0.31660	Н	0.68454	-7.20601	-1.58554
C	-1.38045	-1.26813	-0.56636	C	7.92624	-1.97822	1.22964
C	-2./9/39	-1.32330	-1.04954	C	6.84526	-2.14419	3.4//5/
C	-3.09419	-0.83513	-2.33210	C	7.34114	0.11415	2.46534
	-4.3/955	-0.94640	-2.862/8	H	/.6/542	-3.01926	0.99619
	-5.394/0	-1.54948	-2.11892	п	8.90/92	-1.9/004	1./1090
	-3.11200	-2.04252	-0.04310	п	0.02404	-1.43023	0.20571 1 E4772
U U U	-3.02002	-1.95521	-0.31000	п u	0 2/256	0.11211	2 01116
С	-2.24013	-3.74344	-1.10204	п ц	6 665/1	0.11511	2.91110
с ц	1 20017	5 79829	0 12552	11 11	6 53236	3 17790	3 20007
п	2 40642	-3.68782	0.51120	п н	6 14940	-3.17790 -1.71122	4 20378
н	2 30929		2 29073	н	7 83928	-2 16806	3 94118
н	4.56092	-0.34517	3.24440	C	-7.92630	1.97797	1,22963
C	6 88318		2 16112	C	-6 84529	2 14439	3 47751
н	5,98909	-2.24847	-0.33916	C	-7.34103	-0.11416	2.46566
н	3,73720	-2.16452	-1.27581	н	-7.67556	3.01899	0,99600
н	-2.30921	0.25921	2.29089	н	-8.90797	1.97639	1.71690
н	-4.56083	0.34549	3.24458	Н	-8.02468	1.42982	0.28578
С	-6.88318	1.33213	2.16119	Н	-6.53247	3.17809	3.29073
Н	-5.98919	2.24809	-0.33926	Н	-6.14938	1.71158	4.20377
Н	-3.73733	2.16416	-1.27593	Н	-7.83930	2.16826	3.94113
Н	-2.40642	3.68785	0.51122	Н	-7.37580	-0.71267	1.54814
Н	-1.28815	5.79831	0.12555	Н	-8.34344	-0.11311	2.91150
С	1.21033	6.30172	-0.90854	Н	-6.66525	-0.61599	3.16614

Table	<b>Cable S6.</b> Optimized geometry of the triplet ground state of TBRb at B3LYP/6-31G(d).						
С	0.78101	2.45292	-0.56433	Н	-2.47402	-3.60577	-1.18252
С	1.45469	3.66402	-0.82876	Н	-2.23475	-0.04983	-2.94244
С	0.86933	4.91994	-0.63919	Н	-4.49163	-0.01859	-3.95843
С	-0.44957	4.94367	-0.15577	н	-6.41012	-1.06848	-2.76800
С	-1.15969	3.76990	0.06627	н	-6.03972	-2.14645	-0.55518
С	-0.59463	2.50197	-0.17565	н	-3.78327	-2.17334	0.45219
C	-1.35741	1.27437	-0.08057	Н	2.23484	0.04979	-2.94236
Ċ	-2.74130	1.32958	0.46961	н	4.49179	0.01848	-3.95819
Ċ	-3.01131	0.72893	1.71132	н	6.41024	1.06832	-2.76763
C	-4.27283	0.80861	2,29198	н	6.03971	2.14628	-0.55482
C	-5 33350	1 48558	1 66606	н	3 78319	2 17324	0 45238
C	-5.05910	2.08357	0.42871	C	3.03577	6.00715	-1.46460
C	-3.79282	2.01432	-0.15388	C	1,72001	7.05747	0.38506
C	_0 73406	0 02688	_0 35879	C	0 82463	7 05491	-1 97430
C	0 73401			ч	2 28247	6 50651	1 14752
C	1 35736	-1 27439		н	0 73488	7 29214	0 80176
C	2 7/127	1 32050	0 16962	и 11	2 238/7	8 00627	0 10007
C	2.74127	-1.32930	1 71130	и 11	3 66276	5 /6110	0.75092
C	1 27202	-0.72090	2 2010/	и 11	2 51721	6 07202	1 65500
	4.2/203	1 /0550	1 66600	п 11	2 02011	5 11010	-1.05500
	5 05000	-1.40330	1.00000		2 02576	5.44010 6 00710	-2.40702
	2 70270	-2.00332	0.42007		-3.03370	-0.00718	-1.40407
	5./92/9	-2.01430	-0.15569		-1.72005	-7.05/50	1 07/22
	1 15065	-2.30200	-0.1/502		-0.02401	-7.03494	-1.9/433
	1.13965	-3.70992	0.00030	п	-0./3998	-0.50195	-2.910/8
C	0.44955	-4.943/0	-0.15576	п	-1.33503	-8.00348	-2.18100
C	-0.86934	-4.91997	-0.63921	H	0.18893	-/.28999	-1.63294
C	-1.454/1	-3.66405	-0.828/9	H	-2.28252	-6.50655	1.14/46
C	-0./8104	-2.45295	-0.56434	H	-0./3493	-/.2921/	0.801/4
C	-1.45059	-1.16//2	-0.63801	H	-2.23849	-8.00631	0.19886
C	-2.84330	-1.11383	-1.1/215	Н	-3.662//	-5.46114	-0./5100
C	-3.0/031	-0.50569	-2.41861	H	-3.51/19	-6.9/306	-1.65597
C	-4.34240	-0.48946	-2.98996	H	-3.02808	-5.44821	-2.40/09
C	-5.41/84	-1.08020	-2.324/2	H	0.74003	6.50193	-2.916/5
C	-5.20845	-1.68//8	-1.0848/	H	1.3356/	8.00346	-2.18102
C	-3.93464	-1.70925	-0.51//8	H	-0.18891	/.2899/	-1.63293
C	1.45056	1.16/69	-0.63/98	C	-/./4435	2.32593	1.49948
C	2.84330	1.113//	-1.1/203	C	-6.59600	2.22/95	3./1/82
C	3.0/038	0.50563	-2.4184/	C	-/.25214	0.10103	2.52/4/
C	4.34251	0.48936	-2.989/3	H	-/.43691	3.36/05	1.348/2
C	5.41/92	1.08007	-2.32441	H	-8./104/	2.33864	2.016//
C	5.20846	1.08/05	-1.08458	H	-7.90222	1.8/004	0.51548
C	3.93461	1.70915	-0.51/5/	H	-/.34692	-0.41009	1.56253
H	2.4/401	3.605/4	-1.18246	H	-8.24048	0.11910	3.00336
C	1.61225	6.23684	-0.92272	H	-6.58886	-0.49900	3.15928
H	-0.9428/	5.89145	0.04122	H	-6.22/89	3.25495	3.61284
н	-2.180/1	3.83616	0.4223/	H	-5.90/55	1.69320	4.38048
н	-2.21466	0.19999	2.22/41	Н	-/.5/405	2.2660/	4.21335
Н	-4.42881	0.33289	3.25680	C	7.74436	-2.32580	1.49938
С	-6.71733	1.54052	2.33696	C	6.59606	-2.22779	3.71775
н	-5.83962	2.61273	-0.10697	С	7.25213	-0.10089	2.52733
H	-3.62725	2.47960	-1.12123	H	7.43695	-3.36693	1.34865
H	2.21465	-0.19995	2.22740	H	8.71050	-2.33848	2.01664
Н	4.42882	-0.33279	3.25674	Н	7.90220	-1.86993	0.51537
С	6.71734	-1.54039	2.33686	н	6.22798	-3.25481	3.61280
Н	5.83960	-2.61267	-0.10701	н	5.90763	-1.69304	4.38042
Н	3.62721	-2.47961	-1.12123	н	7.57414	-2.26588	4.21325
Н	2.18067	-3.83618	0.42242	н	7.34687	0.41022	1.56237
Н	0.94284	-5.89147	0.04123	Н	8.24048	-0.11893	3.00320
С	-1.61225	-6.23686	-0.92276	Н	6.58885	0.49915	3.15915

Table	e <b>S7.</b> Optimiz	zed geometry o	of the singlet gro	ound sta	ate of <b>DMeOR</b>	<b>b</b> at B3LYP/6	-31G(d).
С	-0.69539	-3.09066	-0.20286	0	1.20251	5.49585	-0.46012
С	-1.31373	-4.35638	-0.48651	Н	2.35922	3.07452	-0.77576
С	-0.66147	-5.53746	-0.26327	Н	2.34665	-0.26906	-2.56717
С	0.66146	-5.53746	0.26327	Н	4.64755	-0.12268	-3.47193
С	1.31372	-4.35638	0.48652	н	6.46896	0.86445	-2.09110
C	0.69538	-3.09066	0.20287	н	5,95914	1,70418	0.19524
C	1,40219	-1.87359	0.27440	н	3.65571	1.55937	1.08769
C	2.80917	-1.89926	0.78740	н	-2.24851	-0.98935	-2.65658
Ċ	3.06443	-1.41987	2.08226	н	-4.51535	-1.12883	-3.64509
C	4 34122	_1 50032	2 63824	н	_6 38523	-2 12509	-2 33804
	5 38924	-2.06210	1 90742	н	-5 95838	-2.98340	-2.004
C	5 14847	-2.54616	0 62000	н	-3 68905	-2.84706	0 93412
C	3 86950	2 17160	0.06879		2 53387	5 57407	0 0/531
	0 72722	-2.4/100	0.00079		2.53507	5 57407	-0.94531
	0.72732	-0.04084	0.01021	U U	-2.55565	5.57400	1 05/00
	-0./2/32	-0.04004	-0.01021	п	2.74000	0.03044 5.07502	-1.05490
	-1.41281	0.59916	0.21164	п	2.03490	5.07592	-1.91833
C	-2.83821	0.62/51	0.6/256	H	3.24502	5.12636	-0.23894
C	-3.14068	0.15881	1.96114	H	-2./4883	6.63846	1.05491
C	-4.43688	0.24307	2.4/001	H	-2.63494	5.0/593	1.91833
С	-5.45//3	0./9956	1.69/92	Н	-3.24500	5.12638	0.23895
C	-5.17019	1.27371	0.41628				
C	-3.87208	1.19433	-0.08802				
С	-0.70333	1.80914	0.17209				
C	-1.33357	3.07516	0.43646				
C	-0.68154	4.26077	0.24361				
C	0.68155	4.26076	-0.24361				
С	1.33358	3.07515	-0.43647				
С	0.70334	1.80914	-0.17210				
С	1.41281	0.59916	-0.21164				
С	2.83821	0.62752	-0.67256				
С	3.14070	0.15876	-1.96111				
С	4.43690	0.24301	-2.46999				
С	5.45772	0.79957	-1.69792				
С	5.17017	1.27379	-0.41630				
С	3.87207	1.19441	0.08799				
С	-1.40219	-1.87359	-0.27439				
С	-2.80917	-1.89925	-0.78740				
С	-3.06442	-1.41990	-2.08228				
С	-4.34121	-1.50034	-2.63827				
С	-5.38924	-2.06206	-1.90742				
С	-5.14849	-2.54606	-0.61997				
С	-3.86952	-2.47151	-0.06876				
Н	-2.32672	-4.36699	-0.86983				
Н	-1.15786	-6.48057	-0.47640				
Н	1.15785	-6.48057	0.47640				
Н	2.32671	-4.36699	0.86984				
Н	2.24853	-0.98926	2.65654				
Н	4.51537	-1.12876	3.64505				
Н	6.38522	-2.12514	2.33804				
Н	5.95834	-2.98356	0.04184				
Н	3.68901	-2.84720	-0.93407				
Н	-2.34662	-0.26895	2.56722				
Н	-4.64753	-0.12258	3.47197				
Н	-6.46896	0.86443	2.09110				
Н	-5.95917	1.70404	-0.19529				
Н	-3.65573	1.55924	-1.08774				
Н	-2.35921	3.07454	0.77576				
0	-1.20249	5.49585	0.46012				

Table	e <b>S8.</b> Op	timized geometry	of the triplet gro	ound sta	ate of <b>DMeOR</b>	<b>b</b> at B3LYP/6-	-31G(d).
С	0.690	95 1.83765	-0.17506	Н	2.33468	-4.37582	0.81328
С	1.326	41 3.07864	-0.40928	Н	1.17000	-6.50814	0.44012
С	0.673	00 4.29000	-0.22307	Н	-1.16920	-6.50819	-0.44090
С	-0.673	46 4.28992	0.22323	Н	-2.33411	-4.37592	-0.81369
С	-1.326	73 3.07849	0.40947	Н	-2.17942	-0.81790	-2.63472
С	-0.691	12 1.83757	0.17528	Н	-4.41584	-0.89053	-3.69402
С	-1.408	83 0.58270	0.24516	Н	-6.31796	-1.98526	-2.51800
С	-2.813	91 0.59440	0.74958	Н	-5.95221	-3.00510	-0.27740
С	-3.089	15 0.03255	2.00791	Н	-3.71490	-2.93593	0.76957
С	-4.372	24 0.08216	2.55218	Н	2.28267	-0.44048	-2.56126
С	-5.410	27 0.69375	1.84742	Н	4.55928	-0.35418	-3.53012
С	-5.152	69 1.25595	0.59537	Н	6.41106	0.73221	-2.26940
С	-3.867	54 1.21246	0.05556	Н	5.95567	1.72697	-0.03396
С	-0.734	11 -0.64026	-0.01081	Н	3.67862	1.64137	0.92425
С	0.734	28 -0.64018	0.01103	С	-2.57193	5.57337	0.87741
С	1.401	66 -1.86460	0.29389	С	2.57131	5.57367	-0.87726
С	2.783	91 -1.86978	0.85571	н	-2.80643	6.63489	0.97568
С	3.008	13 -1.29458	2.11833	Н	-3.26106	5.11316	0.15702
С	4.268	45 -1.33663	2.71386	Н	-2.69176	5.08137	1.85157
С	5.334	73 -1.95267	2.05667	Н	3.26050	5.11355	-0.15687
С	5.127	89 -2.52787	0.80115	Н	2.80568	6.63521	-0.97555
С	3.865	29 -2.49283	0.21070	Н	2.69121	5.08166	-1.85141
С	0.689	08 -3.12467	0.19944				
С	1.312	56 -4.36224	0.45503				
С	0.654	28 -5.57266	0.24066				
С	-0.653	57 -5.57269	-0.24130				
С	-1.311	98 -4.36230	-0.45546				
С	-0.688	62 -3.12471	-0.19968				
С	-1.401	35 -1.86471	-0.29385				
С	-2.783	64 -1.86993	-0.85559				
С	-3.008	11 -1.29406	-2.11785				
C	-4.268	48 -1.33605	-2.71327				
С	-5.334	55 -1.95272	-2.05635				
C	-5.127	47 -2.52860	-0.80118				
C	-3.864	82 -2.49359	-0.21082				
C	1.408	84 0.58289	-0.24494				
C	2.813	84 0.59481	-0.74957				
С	3.089	05 0.03267	-2.00778				
C	4.372	04 0.08250	-2.55226				
C	5.409	99 0.69461	-1.84786				
C	5.152	44 1.25714	-0.59594				
C	3.867	39 1.21342	-0.05591				
Н	2.358	46 3.07960	-0.72977				
0	1.227	99 5.51585	-0.42527				
0	-1.228	60 5.51571	0.42541				
Н	-2.358	77 3.07933	0.72997				
Н	-2.282	/3 -0.44020	2.56166				
Н	-4.559	51 -0.35427	3.53015				
H	-6.411	42 0.73118	2.26879				
H	-5.955	97 1.72535	0.03311				
H	-3.678	75 1.64014	-0.92472				
H	2.179	28 -0.81892	2.63540				
H	4.415	61 -0.89165	3.69488				
H	6.318	10 -1.98526	2.51840				
H	5.952	/9 -3.00389	0.27718				
Н	3.715	57 -2.93465	-0.76995				

group is replaced with ethyl group) at B3LYP/6-3IG(d).           C         3.44543         -0.69309         -0.21368         H         -1.20166         -3.63404         -1.15635           C         4.71105         -1.30756         -0.50616         H         -2.72070         -2.37197         0.73280           C         5.89235         -0.65594         0.27286         0         -5.14186         -1.21011         0.43642           C         3.44583         0.69114         0.21374         H         0.6162         2.32378         -0.53291         -2.52869           C         2.22803         1.39694         0.29682         H         0.46211         4.70935         -3.39204           C         1.78092         3.02699         2.13511         H         -1.52087         6.50477         -1.797478           C         2.90524         5.13611         0.70808         H         1.49913         -4.44499         -3.27207           C         2.82740         3.80762         0.13355         H         -2.0213         -0.24979         -2.72177         -0.7382         2.49873         -6.34311         -2.48731         -6.34311         -2.48751         -0.8756           C         2.95529         0.72681	Table	e S9. Optimiz	zed geometry	of the singlet g	round s	state of the mo	del of <b>DOcO</b>	<b>Rb</b> (each octyl		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	group	group is replaced with ethyl group) at B3LYP/6-31G(d).								
C       4.71105       -1.30756       -0.50616       H       -2.72070       -2.37197       0.73280         C       5.99273       0.65594       0.27281       0       -5.14115       1.21299       -0.33240         C       3.44583       0.69114       0.21374       H       0.61462       2.39251       -0.53294         C       2.22603       1.39694       0.22062       H       0.46211       4.70935       -3.39204         C       2.225603       2.77490       0.83435       H       -0.52067       6.50477       -1.97478         C       1.78092       3.02699       2.13511       H       -1.35071       5.93350       0.3052         C       2.42549       5.33385       2.00126       H       1.34903       -2.20184       -2.4977         C       0.99529       -0.72681       0.02839       H       -3.3301       -5.95775       -0.14382         C       0.99529       -0.72739       -0.02824       H       3.19899       -3.70679       0.87266         C       0.27547       -2.84968       0.62191       C       -5.23465       -2.58113       0.89752         C       0.27547       -1.46061       2.32253       <	С	3.44543	-0.69309	-0.21368	Н	-1.20166	-3.63404	-1.15635		
C 5.89235 -0.6594 0.27286 0 -5.14186 -1.21011 0.43642 C 5.89235 0.65594 0.27286 0 -5.14186 -1.21011 0.43643 C 4.71181 1.30489 0.50616 H $-2.71929 2.37348 -0.73294 C 2.22890 1.39694 0.29682 H 0.46211 4.70935 -3.39204 C 2.22503 2.79490 0.63435 H -0.52087 6.50477 -1.97478C 1.78092 3.02659 2.13511 H -1.35071 5.9350 0.30552C 1.86467 4.29322 2.71439 H -1.20019 3.63468 1.15605C 2.42549 5.33685 2.00126 H 1.34903 -2.20184 -2.69485C 2.90524 5.13611 0.70808 H 1.49313 -4.44999 -3.70579 0.47266C 0.99559 0.72681 0.02839 H 3.33901 -5.95775 -0.14382C 0.99529 -0.72739 -0.02824 H -5.23455 -2.55813 0.89752C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759C -0.27547 -2.84966 0.62191 C -5.23465 -2.55813 0.89752C 0.18655 -3.17556 1.90712 C -6.70907 -2.88751 -1.05128C 0.09795 -4.48061 2.39253 H -4.70188 2.66141 -1.85464C -0.4552 -5.48659 1.59979 H -4.749473 3.23308 -0.17464C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 -1.05128C -0.24504 -1.41624 0.15949 H -4.70188 2.66141 -1.85464C -2.72111 -1.34062 0.41197 H -7.2285 -2.78039 0.0.9476C -3.90719 -0.68525 0.5.23073 H -4.71087 -2.28855 1.185433C -1.45503 -0.70576 0.15947 H -4.75155 -3.23055 0.17456C -2.72111 -1.34062 0.41197 H -7.2285 -2.78039 0.09476C -3.90719 -0.68726 0.015967 H -4.78172 2.21712 -1.77162C -0.24231 -5.13712 -0.70816C -0.7384 2.84980 -0.62190 H -6.82631 3.92073 -1.40712C -0.27344 2.84980 -0.629671C -0.23254 -2.79618 -0.032452C 2.42210 -1.13283 -0.49314H -7.18072 2.21712 -1.77162C -1.45462 0.70656 -0.15969 H -6.82631 3.92073 -1.40712C -0.27344 2.84980 -0.62951 C -2.82539 -3.86920 -0.13370H -7.22729 2.79175 -0.09337C -1.23454 -0.09485H -0.83579 -1.48956 -0.49314H 4.72261 2.31187 0.90485H 0.45871 -4.79969 3.39222H -0.52744 -6.50458 1.97459H -1.35359 -5.95282 -0.30594$	С	4.71105	-1.30756	-0.50616	Н	-2.72070	-2.37197	0.73280		
C 5.89273 0.65594 0.27286 0 -5.14115 1.21299 0.37348 -0.73294 C 3.44583 0.69114 0.21374 H 0.61462 2.39251 -2.52869 C 2.22800 1.39694 0.29682 H 0.46211 4.70935 -3.39204 C 2.25603 2.79490 0.83435 H -0.52087 6.50477 -1.97478 C 1.78092 3.02699 2.13511 H -1.35071 5.95350 0.30552 C 1.86467 4.29322 2.71439 H -1.20109 3.63468 1.15605 C 2.42549 5.35385 2.00126 H 1.34903 -2.20184 -2.269485 C 2.90524 5.13611 0.70808 H 1.49313 -4.44999 -3.72507 C 2.82740 3.86762 0.13365 H 2.48733 -6.34311 -2.4977 C 0.99559 0.72739 -0.02839 H 3.33901 -5.95775 -0.14382 C 0.99529 -0.72739 -0.02834 H 3.19899 -3.70679 0.87296 C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759 C -0.24504 -1.44061 2.39253 H -4.70188 2.66141 -1.85464 C -0.9559 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.9975 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.45652 -5.48659 1.59979 H -4.74937 3.23308 -0.17464 C -0.42646 -3.86894 -0.15949 H -4.70317 -2.65855 1.85433 C -1.45503 -0.70576 0.15949 H -4.70317 -2.65855 1.85433 C -1.45503 -0.70576 0.15949 H -4.70317 -2.65855 1.85433 C -1.45503 -0.70576 0.15949 H -4.70317 -2.65855 1.85433 C -3.90719 -0.66745 -0.23092 H -6.8227 -3.3105 1.40329 C -2.72031 1.34062 0.41197 H -7.2205 -2.70309 0.09476 C -3.90719 -0.66745 -0.23092 H -6.8227 -3.9105 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -0.24723 1.44626 -0.15969 C -0.43527 5.48677 -1.59993 C -0.27184 2.84980 -0.62190 C 1.84561 -4.292426 -2.71425 C 2.42244 -5.13772 -0.70816 C 2.82549 -3.86920 -0.13370 H 4.72216 -2.31454 -0.90485 H 6.83529 -1.15283 -0.49314 H 6.83599 -1.15283 -0.49314 H 6.83599 -1.15283 -0.49314 H 4.72266 -2.31454 -0.90485 H 6.83529 -1.15283 -0.49314 H 4.72266 -2.31454 -0.90485 H 0.45871 -4.70969 3.39222 H 0.45871 -4.70969 3.39222 H 0.45871 -4.70959 3.39222 H 0.45871 -4.7	C	5.89235	-0.65927	-0.27291	0	-5.14186	-1.21011	0.43642		
C 4.71181 1.30489 0.50016 H $-2.71929$ 2.3748 $-0.73294$ C 3.44583 0.69114 0.21374 H 0.61462 2.39251 $-2.52669$ C 2.22890 1.39694 0.29682 H 0.46211 4.70935 $-3.39204$ C 2.22800 1.39694 0.29682 H $-1.35071$ 5.95350 0.30552 C 1.86467 4.29322 2.71439 H $-1.20193$ 3.63468 1.15605 C 2.42549 5.35385 2.00126 H 1.34903 $-2.20184$ $-2.69485$ C 2.90524 5.13611 0.70808 H 1.49313 $-4.44999$ $-3.72507$ C 0.99559 0.72739 $-0.02824$ H $3.139899$ $-3.70679$ 0.87296 C $-0.24504$ $-1.41614$ 0.18684 C $-5.23315$ 2.56115 $-0.89752$ C $-0.24504$ $-1.41614$ 0.18684 C $-5.23465$ $-2.55813$ 0.89752 C $0.18665$ $-3.17565$ $1.90712$ C $-6.70738$ $2.89157$ $-1.05128$ C $0.09795$ $-4.48061$ $2.39253$ H $-4.70188$ $2.66141$ $-1.85464$ C $-0.45652 -5.48659$ $1.59979$ H $-4.74937$ $3.23308$ $-0.17464$ C $-0.92437$ $-5.17558$ 0.32125 C $-6.70907$ $-2.88751$ $1.05170$ C $-3.90719$ $-0.68252$ 0.23073 H $-7.18095$ $-2.278309$ $0.09476$ C $-2.72031$ $1.34624$ $-0.4197$ H $-7.18095$ $-2.278309$ $0.09476$ C $-3.90719$ $-0.68525$ $0.23073$ H $-7.18075$ $-2.278309$ $0.09476$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18072$ $-2.21712$ $-1.77162$ C $-0.27384$ $2.84677$ $-1.59997$ H $-6.82631$ $3.92073$ $-1.40712$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18072$ $-2.21712$ $-1.77162$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18075$ $-2.21751$ $1.05170$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18072$ $-2.21712$ $-1.77162$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18075$ $-2.21712$ $-1.77162$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18075$ $-2.21751$ $1.40329$ C $-1.45462$ $0.70656$ $-0.158679$ H $-7.22729$ $2.79175$ $-0.09337$ C $-0.27384$ $2.84980$ $-0.62190$ C $1.7784$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42244$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.25474$ $-6.50458$ $1.97459$ H $-0.45871$ $-4.79096$ $3.39222$ H $2.49108$ $6.34174$ $2.44976$ H $3.20071$ $3.70501$ $-0.87308$ H $0.45871$ $-4.70969$ $3.39222$ H $0.45871$ $-4.70969$ $3.39222$ H $0.45871$ $-4.70969$ $3.39222$ H $0.45$	C	5.89273	0.65594	0.27286	0	-5.14115	1.21299	-0.43673		
C 3.44383 0.09114 0.21674 H 0.01462 2.39231 -2.52869 C 2.22800 1.39694 0.29682 H 0.46211 4.70935 -3.39204 C 2.22603 2.79490 0.83435 H -0.52087 6.50477 -1.97478 C 1.78092 3.02699 2.13511 H -1.35071 5.95350 0.30552 C 1.86467 4.29322 2.71439 H -1.20019 3.63468 1.15605 C 2.42549 5.35385 2.00126 H 1.34903 -2.20184 -2.69485 C 2.99524 5.13611 0.70808 H 1.49313 -4.44999 -3.72507 C 2.82740 3.86762 0.13365 H 2.46733 -6.34311 -2.44977 C 0.99559 0.72681 0.02839 H 3.33901 -5.95775 -0.14382 C 0.99559 -0.72739 -0.02824 H 3.19899 -3.70679 0.87296 C -0.24504 -1.41614 0.18664 C -5.2315 2.56115 -0.89759 C -0.27547 -2.84968 0.62191 C -5.23465 -2.55813 0.89752 C 0.18665 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.99759 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.45652 -5.48659 1.59979 H -4.74937 3.23308 -0.17466 C -0.45652 -5.48659 1.59979 H -4.77018 2.26513 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70187 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.77155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90719 -0.68725 0.23073 H -4.18077 -2.65855 1.85443 C -1.45462 0.70556 0.23073 H -7.18075 -2.21561 1.77537 C -0.24423 1.41626 -0.15967 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10033 4.48048 -2.39246 C -0.73275 -2.13612 -0.13370 H -6.83527 -2.13612 -0.79616 C 2.22810 -1.38621 -0.29671 C 2.22810 -1.38622 -0.13370 H 4.72261 2.31187 0.90485 H 6.83529 -1.15283 -0.49314 H 6.83529 -1.15283 -0.49314 H 6.83529 -1.15283 -0.49314 H 4.72261 2.31187 0.90485 H 6.83529 -1.14896 0.49304 H 4.72261 2.31187 0.90485 H 0.45871 -4.70969 3.39222 H 0.45871 -4.70969 3.39222 H -0.45871 -4.70969 3.39294	C	4./1181	1.30489	0.50616	H	-2./1929	2.3/348	-0./3294		
C 2.22830 1.39934 0.29062 H 0.40211 4.0033 -3.39207 C 2.22803 2.79490 0.83435 H $-0.52087$ 6.50477 $-1.97478$ C 1.78092 3.02699 2.13511 H $-1.35071$ 5.95350 0.30552 C 2.42549 5.35385 2.00126 H 1.34903 $-2.20184$ $-2.69485$ C 2.90524 5.13611 0.70808 H 1.49313 $-4.44999$ $-3.72507$ C 2.82740 3.86762 0.13365 H 2.48733 $-6.34311$ $-2.44977$ C 0.99559 0.72739 $-0.02824$ H 3.13989 $-3.70679$ 0.87296 C $-0.24504$ $-1.41614$ 0.18684 C $-5.23315$ 2.56115 $-0.89759$ C $-0.24504$ $-1.41614$ 0.18684 C $-5.23315$ 2.56115 $-0.89759$ C $-0.24504$ $-1.41614$ 0.18684 C $-5.23465$ $-2.55813$ 0.89752 C $0.18665$ $-3.17565$ 1.90712 C $-6.70738$ 2.89157 $-1.05128$ C $0.99759$ $-4.48061$ 2.39253 H $-4.70188$ 2.66141 $-1.85464$ C $-0.45652 -5.48659$ 1.59979 H $-4.770188$ 2.66141 $-1.85464$ C $-0.92437$ $-5.17558$ 0.32125 C $-6.70907$ $-2.88751$ 1.05170 C $-0.84046$ $-3.86894$ $-0.15949$ H $-4.70137$ $-2.65855$ 1.85433 C $-1.45503$ $-0.70576$ 0.15967 H $-4.75155$ $-3.23055$ 0.17456 C $-2.72111$ $-1.34062$ 0.41197 H $-7.22988$ $-2.78309$ 0.09476 C $-2.72013$ 1.34214 $-0.41208$ H $-7.18095$ $-2.21561$ 1.77537 C $-3.90678$ 0.68745 $-0.23072$ H $-6.82873$ $-3.91805$ 1.40329 C $-0.24423$ 1.41626 $-0.18677$ H $-7.22729$ 2.79175 $-0.09337$ C $-0.27342$ 2.84980 $-0.62190$ H $-7.22729$ 2.79175 $-0.09337$ C $-0.24423$ 1.44604 $-2.39246$ C $1.77894$ $-3.02800$ $-2.13493$ C $-0.83857$ 3.86936 0.15930 C $-0.45327$ 5.48677 $-1.59993$ C $-0.24423$ 1.44026 $-2.71425$ C $2.42234$ $-5.35719$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ 2.31187 $0.90485$ H $0.62264$ $-2.39290$ 2.52898 H $0.45871$ $-4.70969$ $3.39222$ H $-0.527474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	3.44583	0.69114	0.213/4	H	0.61462	2.39251	-2.52869		
C 2.2003 2.3020 0.0000 0.0000 0.0000 0.0000 0.000000		2.22890	2 70/00	0.29082	п	0.40211	4.70935	-3.39204		
C 1.7607 C 1.86467 4.29322 2.71439 H -1.20019 3.63468 1.16605 C 2.42549 5.35385 2.00126 H 1.34903 -2.20184 -2.69485 C 2.9524 5.13611 0.70808 H 1.49313 -4.44999 -3.72507 C 0.99569 0.72681 0.02839 H 3.33901 -5.95775 -0.14382 C 0.99529 -0.72739 -0.02824 H 3.19899 -3.70679 0.87296 C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759 C -0.27547 -2.84968 0.62191 C -5.23315 2.56115 -0.89759 C -0.27547 -2.84968 0.62191 C -0.45652 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C -0.45652 -5.48659 1.59979 H -4.74937 3.23308 -0.17464 C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.06170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.105170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.105170 C -3.90719 -0.68525 0.23073 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23924 H -7.18072 -2.21561 1.77537 C -3.90678 0.68745 -0.2392 H -6.82631 3.92073 -1.40329 C -0.47384 2.84980 -0.62190 C -0.445327 5.48677 -1.59993 C -0.27384 2.84980 -0.62190 C -0.45327 5.48677 -1.59993 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C -1.45462 0.70656 -0.15967 H -6.82631 3.92073 -1.40712 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 1.77894 -3.02800 -2.13493 C 2.22810 -1.386921 -0.92671 C 2.22810 -1.386921 -0.92671 C 2.42234 -5.35519 -2.00124 C 2.90246 5.113772 -0.70816 C 2.42234 -5.35519 -2.00124 H 4.72261 2.31187 0.90485 H -6.83529 -1.15283 -0.49314 H 6.83592 -1.15283 -0.49314 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.44234 -5.35519 -1.42842 H -1.35359 -5.95282 -0.30594 H 0.61264 -2.39290 2.52898 H 0.6		2.23003	2.79490	0.03435	п	-0.52087 -1.35071	5 95350	-1.9/4/0		
C 2.42549 5.35385 2.00126 H 1.34903 -2.20184 -2.69485 C 2.90524 5.13611 0.70808 H 1.43313 -4.44999 -3.72507 C 0.99569 0.72681 0.02839 H 2.48733 -6.34311 -2.44977 C 0.99569 0.72739 -0.02824 H 3.19899 -3.70679 0.87296 C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759 C -0.27547 -2.84968 0.62191 C -5.23465 -2.55813 0.89752 C 0.18665 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.09795 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.45652 -5.48659 1.59979 H -4.74937 3.23308 -0.17464 C -0.92437 -5.17558 0.32125 C -6.70937 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.68855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90719 -0.68525 0.23073 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23092 H -6.82673 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -0.24423 1.41626 -0.15569 H -6.82673 -3.91805 1.40329 C -2.72314 2.84980 -0.62190 C -1.4562 0.70556 0.15930 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.5993 C 0.01883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.5993 C 0.22344 -5.35519 -2.01242 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 2.13493 C 0.22343 -5.13772 -0.70816 C 2.82539 -3.86936 0.15930 C 0.24234 -5.13772 -0.70816 C 2.82539 -3.86936 0.15930 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72299 H 2.4108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 0.61264 -2.39290 2.52898 H 0.64564 -2.39290 2.52898 H 0.64567 -4.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	1.86467	4.29322	2.71439	н	-1.20019	3.63468	1.15605		
C       2.90524       5.13611       0.70808       H       1.49313       -4.4999       -3.72507         C       2.82740       3.86762       0.13365       H       2.48733       -6.34311       -2.44977         C       0.99529       -0.72739       -0.02824       H       3.3901       -5.95775       -0.14382         C       0.94529       -0.72739       -0.02824       H       3.19899       -3.70579       0.87296         C       -0.27547       -2.84968       0.62191       C       -5.2315       2.56115       -0.8759         C       0.0795       -4.48061       2.39253       H       -4.70188       2.66141       -1.85464         C       -0.45552       -5.48659       1.59979       H       -4.70188       2.66141       -1.185464         C       -0.92437       -5.17556       0.32125       C       -6.70937       3.23308       -0.17464         C       -0.84046       -3.86894       -0.15949       H       -4.74937       3.23308       -0.17464         C       -2.72111       -1.34062       0.41197       H       -7.22855       1.85443         C       -1.45503       -0.70706       0.15949       H	c	2.42549	5.35385	2.00126	н	1.34903	-2.20184	-2.69485		
C 2.82740 3.86762 0.13365 H 2.48733 -6.34311 -2.44977 C 0.99569 0.72681 0.02839 H 3.33901 -5.95775 -0.14382 C 0.99529 -0.72739 -0.02824 H 3.19899 -3.70679 0.87296 C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759 C -0.27547 -2.84968 0.6219 C -5.23465 -2.55813 0.89752 C 0.18665 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.09795 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.70517 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -0.24423 1.41626 -0.15969 H -6.8263 3.92073 -1.40712 C -0.24423 1.41626 -0.16877 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 H -6.82631 3.92073 -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 H -6.8261 3.92073 -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 H -6.8261 3.92073 -1.40712 C -0.24423 -1.5128 -0.90485 H 6.8352 -1.15283 -0.49314 H 6.8359 1.14896 0.49304 H 4.72126 -2.31454 -0.90485 H 6.8352 -1.15283 -0.49314 H 6.8359 1.14895 0.41393 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35719 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	2.90524	5.13611	0.70808	Н	1.49313	-4.44999	-3.72507		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	2.82740	3.86762	0.13365	Н	2.48733	-6.34311	-2.44977		
C       0.99529       -0.72739       -0.02824       H       3.19899       -3.70679       0.87296         C       -0.24504       -1.41614       0.18684       C       -5.23315       2.56115       -0.89759         C       0.18665       -3.17565       1.90712       C       -6.70738       2.89157       -1.05128         C       0.045652       -5.48659       1.59979       H       -4.70188       2.66141       -1.85464         C       -0.42637       -5.17558       0.32125       C       -6.70907       -2.88751       1.05170         C       -0.84046       -3.68894       -0.15949       H       -4.70188       2.32055       0.17464         C       -2.8406       0.67756       0.15967       H       -4.70317       -2.68751       1.05170         C       -3.90718       0.68745       -0.23092       H       -4.70185       -3.23055       0.17456         C       -2.72031       1.34214       -0.41208       H       -7.18095       -2.21561       1.77537         C       -0.27384       2.84980       -0.62190       H       -6.82631       3.92073       -1.40712         C       -0.43237       5.35519       -2.01	С	0.99569	0.72681	0.02839	Н	3.33901	-5.95775	-0.14382		
C -0.24504 -1.41614 0.18684 C -5.23315 2.56115 -0.89759 C -0.27547 -2.84968 0.62191 C -5.23465 -2.55813 0.89752 C 0.18665 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.09795 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.45652 -5.48659 1.59979 H -4.7497 3.22308 -0.17464 C -0.84046 -3.86894 -0.15949 H -4.7497 3.223055 0.17456 C -2.72111 -1.34062 0.41197 H -4.75155 -3.23055 0.17456 C -2.72011 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90678 0.68745 -0.23092 H -6.8273 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23092 H -6.8273 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.45327 5.48677 -1.59993 C -0.45327 5.48677 -1.59993 C -0.22168 5.17603 -0.32152 C -0.453527 5.48677 -1.59993 C -0.45327 5.48677 -1.59993 C -0.24246 -5.13772 -0.70816 C 2.22810 -1.39821 -0.29671 C 2.22842 -3.55519 -2.01024 C 2.90246 -5.13772 -0.70816 C 2.202549 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83552 -1.15283 -0.49314 H 6.83599 1.14986 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.34210 5.95591 0.14364 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.977459 H -1.35359 -5.95282 -0.30594	С	0.99529	-0.72739	-0.02824	Н	3.19899	-3.70679	0.87296		
C -0.27547 -2.84968 0.62191 C -5.23465 -2.55813 0.89752 C 0.18665 -3.17565 1.90712 C -6.70738 2.89157 -1.05128 C 0.09795 -4.48061 2.39253 H -4.70188 2.66141 -1.85464 C -0.45652 -5.48659 1.59979 H -4.70188 2.66141 -1.85464 C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.21861 1.77537 C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18095 -2.21561 1.77537 C -0.27384 2.84980 -0.62190 H -6.82631 3.92073 -1.40712 C -0.27384 2.84960 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.92168 5.17603 -0.21902 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.213493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83592 1.14826 0.49304 H 4.72261 2.31187 0.90485 H 6.83592 1.14895 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.34210 5.95591 0.14364 H 0.61264 -2.39290 2.52898 H 0.61264 -2.39290 2.52898 H 0.61264 -2.39290 2.52898 H 0.65274 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	-0.24504	-1.41614	0.18684	C	-5.23315	2.56115	-0.89759		
C 0.18665 $-3.17565$ 1.90712 C $-6.70738$ 2.89157 $-1.05128$ C 0.09795 $-4.48061$ 2.39253 H $-4.70188$ 2.66141 $-1.85464$ C $-0.92437$ $-5.17558$ 0.32125 C $-6.70907$ $-2.88751$ 1.05170 C $-0.84046$ $-3.86894$ $-0.15949$ H $-4.70187$ 2.26555 1.85443 C $-1.45503$ $-0.70576$ 0.15967 H $-4.75155$ $-3.23055$ 0.17456 C $-2.72111$ $-1.34062$ 0.41197 H $-7.22985$ $-2.78309$ 0.09476 C $-3.90719$ $-0.68525$ 0.23073 H $-7.18072$ 2.21712 $-1.77537$ C $-3.90678$ 0.68745 $-0.23092$ H $-6.82873$ $-3.91805$ 1.40329 C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18072$ 2.21712 $-1.77162$ C $-0.24423$ $1.41626$ $-0.18677$ H $-7.22729$ $2.79175$ $-0.09337$ C $-0.27384$ 2.84980 $-0.62190$ H $-6.82631$ $3.92073$ $-1.40712$ C $-0.45327$ $5.48677$ $-1.59993$ C $0.10093$ $4.48048$ $-2.39246$ C $0.10093$ $4.48048$ $-2.39246$ C $0.10093$ $4.48048$ $-2.39246$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83592$ $-1.15283$ $-0.49314$ H $4.72126$ $-2.31454$ $-0.90485$ H $4.72126$ $-2.31454$ $-0.90485$ H $4.72126$ $-2.31454$ $-0.90485$ H $4.72126$ $2.31187$ $0.90485$ H $4.72126$ $-2.319591$ $-1.48976$ H $4.72164$ $-2.39290$ $2.52898$ H $0.61264$ $-2.39290$ $2.52898$ H $0.61264$ $-2.39290$ $2.52898$ H $0.65871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.977459$ H $-1.35359$ $-5.95282$ $-0.30594$	С	-0.27547	-2.84968	0.62191	C	-5.23465	-2.55813	0.89752		
C $0.09795 - 4.48061 2.39253 H - 4.70188 2.66141 -1.85464 C -0.45652 - 5.48659 1.59979 H -4.74937 3.23308 -0.17464 C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456C -2.77111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90719 -0.68525 0.23073 H -7.18095 -2.21561 1.77537C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162C -0.24423 1.41626 -0.15969 H -6.82631 3.92073 -1.40712C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337C -0.27384 2.84980 -0.62190C 0.18883 3.17549 -1.90698C 0.10093 4.48048 -2.39246C -0.45327 5.48677 -1.59993C -0.92168 5.17603 -0.32152C -0.83857 3.86936 0.15930C 2.22810 -1.39821 -0.29671C 2.22842 -2.79618 -0.83426C 1.77894 -3.02800 -2.13493C 1.86191 -4.29426 -2.71425C 2.42234 -5.35519 -2.00124H 4.72126 -2.31454 -0.90485H 4.72261 2.31187 0.90485H 4.72261 2.31187 0.90485H 1.35070 2.20106 2.69512H 1.49616 4.44915 3.72529H 2.49108 6.34174 2.44976H 3.34210 5.95591 0.14364H 3.20071 3.70501 -0.87308H 0.61264 -2.39290 2.52898H 0.645871 -4.70969 3.39222H -0.52474 -6.50458 1.97459$	С	0.18665	-3.17565	1.90712	С	-6.70738	2.89157	-1.05128		
C -0.45652 -5.48659 1.59979 H $-4.74937$ 3.23308 -0.17464 C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H $-4.70317$ -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H $-4.775155$ -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H $-7.22985$ -2.78309 0.09476 C -3.90078 0.68745 -0.23092 H $-6.82873$ -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H $-7.18095$ -2.21712 -1.77162 C -1.45462 0.70656 -0.15969 H $-6.82631$ 3.92073 -1.40712 C -0.27384 2.84980 -0.62190 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.225442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 $-4.29426$ -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.772126 -2.31454 -0.90485 H 6.83532 -1.15283 -0.49314 H 6.83599 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.39071 3.70501 -0.87308 H 0.61264 -2.392920 -2.52898 H 0.642641 -2.392920 -2.52898 H 0.64264 -2.39290 2.52898 H 0.643671 -4.70969 3.39222	C	0.09795	-4.48061	2.39253	Н	-4.70188	2.66141	-1.85464		
C -0.92437 -5.17558 0.32125 C -6.70907 -2.88751 1.05170 C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90678 0.68745 -0.23073 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.83857 3.86936 0.15930 C 2.22840 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.82539 -3.86920 -0.13370 H 4.77126 -2.31454 -0.90485 H 6.83592 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.65912 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	-0.45652	-5.48659	1.59979	Н	-4.74937	3.23308	-0.17464		
C -0.84046 -3.86894 -0.15949 H -4.70317 -2.65855 1.85443 C -1.45503 -0.70576 0.15967 H -4.75155 -3.23055 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90719 -0.68525 0.23073 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -1.45462 0.70656 -0.15969 H -6.82631 3.92073 -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 H 6.83539 -1.14286 0.49314 H 6.83599 1.14896 0.49314 H 6.83599 1.14896 0.49314 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	-0.92437	-5.17558	0.32125	C	-6.70907	-2.88751	1.05170		
C -1.43503 -0.70576 0.13967 H -4.75155 -5.72305 0.17456 C -2.72111 -1.34062 0.41197 H -7.22985 -2.78309 0.09476 C -3.90678 0.68745 -0.23092 H -7.18095 -2.21561 1.77537 C -3.90678 0.68745 -0.23092 H -6.82637 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -1.45462 0.70656 -0.15969 H -6.82631 3.92073 -1.40712 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83522 -1.15283 -0.49314 H 6.83532 -1.15283 -0.49314 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.61264 -2.39290 2.52899 H -0.52474 -6.50458 1.97459 H -0.52474 -6.	C	-0.84046	-3.86894	-0.15949	H	-4./031/	-2.65855	1.85443		
C $-2.72111$ $-1.34062$ $0.41137$ H $-7.72303$ $-2.7503$ $-2.7503$ C $-3.90719$ $-0.68525$ $0.23073$ H $-7.18095$ $-2.21561$ $1.77537$ C $-3.90678$ $0.68745$ $-0.23092$ H $-6.82873$ $-3.91805$ $1.40329$ C $-2.72031$ $1.34214$ $-0.41208$ H $-7.18072$ $2.21712$ $-1.77162$ C $-1.45462$ $0.70656$ $-0.15969$ H $-6.82631$ $3.92073$ $-1.40712$ C $-0.24423$ $1.41626$ $-0.18677$ H $-7.22729$ $2.79175$ $-0.09337$ C $-0.27384$ $2.84980$ $-0.62190$ C $0.10893$ $3.17549$ $-1.90698$ C $0.10093$ $4.48048$ $-2.39246$ C $-0.45327$ $5.48677$ $-1.59993$ C $-0.92168$ $5.17603$ $-0.32152$ C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.255442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.33290$ $2.52898$ H $0.61264$ $-2.33290$ $2.52898$ H $0.652474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	-1.45503	-0.70576	0.15967	H	-4./5155	-3.23055	0.1/456		
C -3.90678 0.68745 -0.23092 H -6.82873 -3.91805 1.40329 C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -1.45462 0.70656 -0.15969 H -6.82631 3.92073 -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83592 -1.15283 -0.49314 H 6.83592 -1.15283 -0.49314 H 6.83592 -1.15283 -0.49314 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.61264 -2.3929		-2./2111	-1.34062	0.41197	п	-/.22985	-2./8309	0.094/0		
C -2.72031 1.34214 -0.41208 H -7.18072 2.21712 -1.77162 C -1.45462 0.70656 -0.15969 H -6.82631 $3.92073$ -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 $3.17549$ -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 $3.86936$ 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83552 -1.15283 -0.49314 H 6.83599 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594		-3.90/19	-0.08525	0.23073	п ц	-7.10095	-2.21301	1 /0329		
C -1.145462 0.70656 -0.15969 H -6.82631 3.92073 -1.40712 C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83532 -1.15283 -0.49314 H 6.83599 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	-2 72031	1 34214		н	-7 18072	2 21712	_1 77162		
C -0.24423 1.41626 -0.18677 H -7.22729 2.79175 -0.09337 C -0.27384 2.84980 -0.62190 C 0.18883 3.17549 -1.90698 C 0.10093 4.48048 -2.39246 C -0.45327 5.48677 -1.59993 C -0.92168 5.17603 -0.32152 C -0.83857 3.86936 0.15930 C 2.22810 -1.39821 -0.29671 C 2.25442 -2.79618 -0.83426 C 1.77894 -3.02800 -2.13493 C 1.86191 -4.29426 -2.71425 C 2.42234 -5.35519 -2.00124 C 2.90246 -5.13772 -0.70816 C 2.82539 -3.86920 -0.13370 H 4.72126 -2.31454 -0.90485 H 6.83592 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 -0.87308 H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	C	-1.45462	0.70656	-0.15969	н	-6.82631	3,92073	-1.40712		
C $-0.27384$ 2.84980 $-0.62190$ C $0.18883$ $3.17549$ $-1.90698$ C $0.10093$ $4.48048$ $-2.39246$ C $-0.45327$ $5.48677$ $-1.59993$ C $-0.92168$ $5.17603$ $-0.32152$ C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	-0.24423	1,41626	-0.18677	н	-7.22729	2.79175	-0.09337		
C 0.18883 $3.17549 -1.90698$ C 0.10093 $4.48048 -2.39246$ C $-0.45327 5.48677 -1.59993$ C $-0.92168 5.17603 -0.32152$ C $-0.83857 3.86936 0.15930$ C $2.22810 -1.39821 -0.29671$ C $2.25442 -2.79618 -0.83426$ C $1.77894 -3.02800 -2.13493$ C $1.86191 -4.29426 -2.71425$ C $2.42234 -5.35519 -2.00124$ C $2.90246 -5.13772 -0.70816$ C $2.82539 -3.86920 -0.13370$ H $4.72126 -2.31454 -0.90485$ H $6.83532 -1.15283 -0.49314$ H $6.83599 1.14896 0.49304$ H $4.72261 2.31187 0.90485$ H $1.35070 2.20106 2.69512$ H $1.49616 4.44915 3.72529$ H $2.49108 6.34174 2.44976$ H $3.20071 3.70501 -0.87308$ H $0.61264 -2.39290 2.52898$ H $0.45871 -4.70969 3.39222$ H $-0.52474 -6.50458 1.97459$ H $-1.35359 -5.95282 -0.30594$	C	-0.27384	2.84980	-0.62190						
C $0.10093$ $4.48048$ $-2.39246$ C $-0.45327$ $5.48677$ $-1.59993$ C $-0.92168$ $5.17603$ $-0.32152$ C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	0.18883	3.17549	-1.90698						
C $-0.45327$ $5.48677$ $-1.59993$ C $-0.92168$ $5.17603$ $-0.32152$ C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	С	0.10093	4.48048	-2.39246						
C $-0.92168$ $5.17603$ $-0.32152$ C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	С	-0.45327	5.48677	-1.59993						
C $-0.83857$ $3.86936$ $0.15930$ C $2.22810$ $-1.39821$ $-0.29671$ C $2.25442$ $-2.79618$ $-0.83426$ C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.4915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	С	-0.92168	5.17603	-0.32152						
C 2.22810 $-1.39821$ $-0.29671$ C 2.25442 $-2.79618$ $-0.83426$ C 1.77894 $-3.02800$ $-2.13493$ C 1.86191 $-4.29426$ $-2.71425$ C 2.42234 $-5.35519$ $-2.00124$ C 2.90246 $-5.13772$ $-0.70816$ C 2.82539 $-3.86920$ $-0.13370$ H 4.72126 $-2.31454$ $-0.90485$ H 6.83532 $-1.15283$ $-0.49314$ H 6.83599 1.14896 0.49304 H 4.72261 2.31187 0.90485 H 1.35070 2.20106 2.69512 H 1.49616 4.44915 3.72529 H 2.49108 6.34174 2.44976 H 3.34210 5.95591 0.14364 H 3.20071 3.70501 $-0.87308$ H 0.61264 $-2.39290$ 2.52898 H 0.45871 $-4.70969$ 3.39222 H $-0.52474$ $-6.50458$ 1.97459 H $-1.35359$ $-5.95282$ $-0.30594$	С	-0.83857	3.86936	0.15930						
C $2.25442 -2.79618 -0.83426$ C $1.77894 -3.02800 -2.13493$ C $1.86191 -4.29426 -2.71425$ C $2.42234 -5.35519 -2.00124$ C $2.90246 -5.13772 -0.70816$ C $2.82539 -3.86920 -0.13370$ H $4.72126 -2.31454 -0.90485$ H $6.83532 -1.15283 -0.49314$ H $6.83599 1.14896 0.49304$ H $4.72261 2.31187 0.90485$ H $1.35070 2.20106 2.69512$ H $1.49616 4.44915 3.72529$ H $2.49108 6.34174 2.44976$ H $3.34210 5.95591 0.14364$ H $3.20071 3.70501 -0.87308$ H $0.61264 -2.39290 2.52898$ H $0.45871 -4.70969 3.39222$ H $-0.52474 -6.50458 1.97459$ H $-1.35359 -5.95282 -0.30594$	C	2.22810	-1.39821	-0.29671						
C $1.77894$ $-3.02800$ $-2.13493$ C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	2.25442	-2.79618	-0.83426						
C $1.86191$ $-4.29426$ $-2.71425$ C $2.42234$ $-5.35519$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	1.77894	-3.02800	-2.13493						
C $2.42234$ $-5.33319$ $-2.00124$ C $2.90246$ $-5.13772$ $-0.70816$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	C	1.86191	-4.29426	-2./1425						
C $2.90240$ $-3.13772$ $-0.70010$ C $2.82539$ $-3.86920$ $-0.13370$ H $4.72126$ $-2.31454$ $-0.90485$ H $6.83532$ $-1.15283$ $-0.49314$ H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$		2.42234	-3.33319 5 12772	-2.00124 0 70016						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		2.90240	-3.86920	-0.13370						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	н	4,72126	-3.31454	-0.90485						
H $6.83599$ $1.14896$ $0.49304$ H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	н	6.83532	-1.15283	-0.49314						
H $4.72261$ $2.31187$ $0.90485$ H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	6.83599	1.14896	0.49304						
H $1.35070$ $2.20106$ $2.69512$ H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	4.72261	2.31187	0.90485						
H $1.49616$ $4.44915$ $3.72529$ H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	1.35070	2.20106	2.69512						
H $2.49108$ $6.34174$ $2.44976$ H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	1.49616	4.44915	3.72529						
H $3.34210$ $5.95591$ $0.14364$ H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	2.49108	6.34174	2.44976						
H $3.20071$ $3.70501$ $-0.87308$ H $0.61264$ $-2.39290$ $2.52898$ H $0.45871$ $-4.70969$ $3.39222$ H $-0.52474$ $-6.50458$ $1.97459$ H $-1.35359$ $-5.95282$ $-0.30594$	Н	3.34210	5.95591	0.14364						
H 0.61264 -2.39290 2.52898 H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	Н	3.20071	3.70501	-0.87308						
H 0.45871 -4.70969 3.39222 H -0.52474 -6.50458 1.97459 H -1.35359 -5.95282 -0.30594	Н	0.61264	-2.39290	2.52898						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	H	0.45871	-4.70969	3.39222						
н –1.35359 –5.95282 –0.30594	H	-0.52474	-6.50458	1.97459						
	н	-1.33339	-3.95282	-0.30394						

Table	S10. Optim	nized geometry	of the triplet g	round	state of the mo	odel of <b>DOcO</b>	<b>Rb</b> (each octyl	
group	group is replaced with ethyl group) at B3LYP/6-31G(d).							
С	-3.47866	0.68401	-0.21282	Н	2.72438	2.36919	0.69713	
C	-4.71651	1.30203	-0.47994	0	5.16086	1.23575	0.40842	
C	-5.92665	0.64761	-0.25294	0	5.16161	-1.23260	-0.40856	
C	-5.92622	-0.65115	0.25340	H	2./2583	-2.36/51	-0.69/32	
C	-4./1505	-1.30483	0.48025	H	-0.81/39	-2.31555	-2.51/65	
C	-3.4/022	-0.00004	0.21290	п ц	-0.74454	-4.00303	-3.43070	
c	$-2 \cdot 21794$ $-2 \cdot 21818$	-2 76517	0.91442	н	1 37246	-5 95691	0 03545	
C	-1.63031	-2.95830	2.17652	н	1.29923	-3.66726	0.96407	
c	-1.66317	-4.20408	2.80226	Н	-1.15420	2.11552	-2.66975	
C	-2.28298	-5.28712	2.17667	Н	-1.21206	4.32585	-3.78267	
С	-2.87057	-5.11143	0.92220	Н	-2.31307	6.25797	-2.66197	
С	-2.84429	-3.86319	0.30120	Н	-3.35232	5.94791	-0.42211	
С	-0.99427	-0.73390	0.02342	Н	-3.29586	3.73675	0.67957	
С	-0.99471	0.73336	-0.02364	С	5.23405	-2.58936	-0.84489	
С	0.22770	1.41242	0.22363	С	5.23247	2.59253	0.84484	
С	0.23480	2.82368	0.71010	С	6.70429	-2.94293	-0.98745	
C	-0.34160	3.11485	1.95834	H	4.70679	-2.70180	-1.80286	
C	-0.29985	4.40498	2.48632	H	4.74088	-3.24414	-0.11227	
C	0.31842	5.43453	1.//482	C T	6.70249	2.94697	0.98/48	
C	0.89498	5.1011/ 2.06001	0.532/3	H U	4.70510	2.70460	1.802/9	
C	1 10200	0 60200	0.16520	п u	4.73094	J.24/00	0.02010	
c	2 72351	1 33304	0.10559	п н	7 18687	2.03437	1 71975	
c	3,93569	0.67771	0.21390	н	6.80823	3.98472	1,32191	
C	3,93610	-0.67531	-0.21405	н	7,18831	-2.28931	-1.71975	
C	2.72433	-1.33137	-0.39101	Н	6.81067	-3.98064	-1.32181	
C	1.48322	-0.69306	-0.16558	н	7.22238	-2.82995	-0.03005	
С	0.22854	-1.41224	-0.22383					
С	0.23644	-2.82355	-0.71014					
С	-0.33951	-3.11514	-1.95850					
С	-0.29703	-4.40531	-2.48630					
C	0.32150	-5.43450	-1.77451					
C	0.89759	-5.16073	-0.53229					
C	0.86115	-3.86852	-0.00903					
C	-2.21882	1.39508	-0.32069					
C	-2.21990 -1.63277	2.70300	-0.91451 -2.17688					
c	-1.66654	4,20299	-2.80266					
c	-2.28661	5.28575	-2.17684					
C	-2.87354	5.10982	-0.92209					
С	-2.84636	3.86161	-0.30106					
Н	-4.73035	2.31705	-0.85785					
Н	-6.86235	1.15913	-0.46196					
Н	-6.86158	-1.16325	0.46253					
Н	-4.72881	-2.31987	0.85814					
H	-1.15193	-2.11634	2.66920					
H	-1.20818	-4.32675	3.78205					
H	-2.308/4	-0.25938	2.001/8 0.42240					
н ч	-3.34910 _3.20/20	-3.349/4 _3.73051	0.42240					
л म	-3.23429	- 3 • 7 3 6 5 I 2 3 1 4 9 9	-0.0/921 2 51726					
н	-0.74772	4,60439	3.45668					
н	0.34992	6.44126	2.18320					
H	1.36966	5.95763	-0.03477					
Н	1.29773	3.66807	-0.96369					
	-							