Electronic Supplementary Information

Cationic Half-Sandwich Quinolinophaneoxazoline-Based (η⁶-p-Cymene)ruthenium(II) Complexes Exhibiting Different Chirality Types: Synthesis, and Structural Determination by Complementary Spectroscopic Methods

Renzo Ruzziconi, * ^a Gianfranco Bellachioma, ^a Gianluca Ciancaleoni, ^a Susan Lepri, ^a Stefano Superchi, *^b Riccardo Zanasi, *^c and Guglielmo Monaco ^c

^a Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy

^b Dipartimento di Scienze, Università della Basilicata, Viale dell'Ateneo Lucano 10, 85100 Potenza, Italy.

^c Dipartimento di Chimica e Biologia, Università di Salerno, via Ponte Don Melillo Fisciano, 84084 (SA), Italy

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$[(R_p, R, R_{Ru})-[Ru(\eta^6-p-cymene)(QUIPHANEPHOX)Cl]^+BPh_4^-(6a)$

$$[\alpha]_D^{20} = +298 \ (c = 0.1, \text{CHCl}_3)$$



Table S1. Chemical shift values assigned to the protons of complex (R_p, R, R_{Ru}) -6a in CDCl₃

H-3 (s)	7.84	H-22t (<i>t</i>)	4.92
H-6 (d_{AB})	7.07	H-23 (<i>t</i>)	5.22
H-7 (d_{AB})	7.16	H-25 (broad)	5.05
H-9a (<i>dt</i>)	3.09	H-25' (<i>d</i>)	4.77
H-9s (<i>m</i>)	5.59	H-26 (<i>d</i>)	5.05
H-10a (<i>m</i>)	2.87	H-26'	4.82
H-10s (<i>m</i>)	3.22	H-28 (broad)	1.5
H-12 (dd_{AB})	6.61	H-29 (<i>d</i>)	0.43
H-13 (dd_{AB})	6.74	H-29'(broad)	0.44
H-15 (<i>dd</i>)	5.56	H-31 (broad)	1.5
H-16 (<i>dd</i>)	5.56	H-32 (<i>o</i>)	7.4
H-17a (<i>dt</i>)	3.34	H-33 (<i>m</i>)	7.4
H-17s (<i>dd</i>)	2.84	H-34 (<i>p</i>)	7.4
H-18a (<i>dd</i>)	3.2	BPh ₄ o (8 H)	7.4
H-18s (<i>ddd</i>)	4.00	BPh4 <i>m</i> (8 H)	7.0
H-19 (s)	3.02	$BPh_4 p (t, 4 H)$	6.90
H-22c (<i>dd</i>)	4.47		





$[(R_p, R, R_{Ru}) - [Ru(\eta^6 - p - cymene)(QUIPHANEPHOX)Cl]^+ PF_6^- (6b)$



H-3 (<i>s</i>)	7.90	H-19 (s)	3.09
H-6 (d_{AB})	7.08	H-22c (<i>dd</i>)	4.73
H-7 (d_{AB})	7.23	H-22t (<i>dd</i>)	5.60
H-9a (<i>m</i>)	3.2	H-23 (<i>t</i>)	6.30
H-9s (<i>m</i>)	5.73	H-25 (<i>d</i>)	5.25
H-10a (<i>m</i>)	2.92	H-25' (<i>d</i>)	5.79
H-10s (<i>m</i>)	3.30	H-26 (<i>d</i>)	5.13
H-12 (dd_{AB})	6.63	H-26' (<i>d</i>)	5.73
H-13 (<i>dd</i> _{AB})	6.75	H-28 (broad)	1.7
H-15 (<i>dd</i>) _{AB}	5.58	H-29 (<i>d</i>)	0.51
H-16 (<i>dd</i>) _{AB}	5.66	H-29'(broad)	0.56
H-17a (<i>m</i>)	3.38	H-31 (broad s)	1.25
H-17s (<i>dd</i>)	2.88	H-32 (<i>o</i>)	7.73
H-18a (<i>dd</i>)	3.20	H-33 (<i>m</i>)	7.5
H-18s (<i>dt</i>)	4.09	H-34 (<i>p</i>)	7.50

Table S2. Chemical shift values assigned to the protons of complex (R_p, R, R_{Ru}) -6b in CDCl₃.



Figure S1. A section of the ¹H-NOESY diagram (400.13MHz, 293 K,CDCl₃) for complex **6b** showing the NOE correlations of the *p*-cymene aromatic protons H-27 and H-28 with H-23 of the oxazoline ring.







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$[(R_p, S, R_{Ru})-[Ru(\eta^6-p-cymene)(QUIPHANEPHOX)Cl]^+BPh_4 (7a)$

$$[\alpha]_{D}^{20} = +514 \ (c = 0.081, CHCl_3)$$



Table S3. Chemical shift values assigned to the protons of complex (R_p, S, R_{Ru}) -7a in CDCl₃.

H-3 (s)	7.75	H-22t (<i>t</i>)	4.93
H-6 (d_{AB})	7.03	H-23 (<i>t</i>)	5.52
H-7 (d_{AB})	7.08	H-25 (very broad)	n.d.
H-9a (<i>dt</i>)	3.07	H-25' (very broad)	n.d.
H-9s (<i>m</i>)	5.31	H-26 (very broad)	n.d.
H-10a (<i>m</i>)	2.90	H-26' (very broad)	n.d.
H-10s (<i>m</i>)	3.05	H-28 (very broad)	~ 2.0
H-12 (dd_{AB})	6.58	H-29 (very broad)	0.4
H-13 (dd_{AB})	6.70	H-29' (very broad)	0.4
H-15 (<i>dd</i>)	5.50	H-31 (very broad)	~ 1.2
H-16 (<i>dd</i>)	5.43	H-32 (<i>o</i>)	7.4
H-17a (<i>dt</i>)	3.34	H-33 (<i>m</i>)	7.4
H-17s (<i>dd</i>)	2.80	H-34 (<i>p</i>)	7.4
H-18a (<i>dd</i>)	3.17	BPh ₄ <i>o</i> (m, 8 H)	7.39
H-18s (<i>ddd</i>)	3.97	BPh ₄ <i>m</i> (t, 8 H)	6.96
H-19 (s)	2.93	BPh ₄ <i>p</i> (t, 4 H)	6.85
H-22c(t)	5.27		

¹H (400 MHz)

C63H60BCIN2Ru



$[(R_p, S, R_{Ru})-[Ru(\eta^6-p-cym)(QUIPHANEPHOX)Cl]^+BPh_4(CD_2Cl_2) (7a)$



Table S4. Chemical shift values assigned to the protons of complex (R_p, S, R_{Ru}) -7a in CD₂Cl₂.

H-3 (s)	7.90	H-22c (<i>dd</i>)	5.42
H-6 (d_{AB})	7.17	H-23 (<i>dd</i>)	5.62
H-7 (d_{AB})	7.28	H-25 (very broad)	3.9
H-9a (<i>dt</i>)	3.18	H-25' (very broad)	~4.3
H-9s (<i>m</i>)	5.43	H-26 (very broad)	~5.1
H-10a (<i>m</i>)	2.96	H-26'	n.d.
H-10s (<i>m</i>)	3.10	H-28 (very broad)	1.3
H-12 (dd_{AB})	6.65	H-29 (very broad)	0.1
H-13 (dd_{AB})	6.77	H-29' (very broad)	0.4
H-15 (<i>dd</i>)	5.59	H-31 (very broad)	2.3
H-16 (<i>dd</i>)	5.47	H-32 <i>o</i> (<i>m</i>)	7.6
H-17a (<i>dt</i>)	3.40	H-33 m (m)	7.7
H-17s (<i>dd</i>)	2.88	H-34 <i>p</i> (<i>m</i>)	7.7
H-18a (<i>dd</i>)	3.26	BPh ₄ o (8 H)	7.3
H-18s (ddd)	4.06	BPh ₄ <i>m</i> (8 <i>H</i>)	7.05
H-19(s)	3.07	$BPh_4 p (t, 4 H)$	6.9
H-22t (<i>dd</i>)	5.05		



Figure S2. A section of the ¹H-NOESY (400.13MHz, 293 K,CDCl₃) for complex **7a** showing NOE between aromatic protons H-24 of the phenyl ring and both H-23 and H-22t. No NOE correlation is observed involving either *p*-cymene or BPh₄ aromatic protons.



$[(R_p, S, R_{Ru})-[Ru(\eta^6-p-cymene)(QUIPHANEPHOX)Cl]^+PF_6^-(7b)$



Table S5. Chemical shift values assigned to the protons of complex (R_p, S, R_{Ru}) -7b.

H-3 (s)	8.12	H-19 (<i>s</i>)	3.09
H-6 (d_{AB})	7.10	H-22c (<i>t</i>)	5.36
H-7 (<i>d</i> _{AB})	7.23	H-22t (<i>t</i>)	5.16
H-9a (<i>dt</i>)	3.16	H-23 (<i>t</i>)	5.56
H-9s (<i>m</i>)	5.49	H-25 (very broad)	~4.9
H-10a (<i>m</i>)	2.93	H-25'	~4.9
H-10s (<i>m</i>)	3.18	H-26 (very broad)	~5.2
H-12 (dd_{AB})	6.60	H-26'	~5.2
H-13 (<i>dd</i> _{AB})	6.71	H-28	n.d.
H-15 (<i>dd</i>)	5.58	H-29 (<i>b</i>)	1.0
H-16 (<i>dd</i>)	5.51	H-29'(<i>d</i>)	1.0
H-17a (<i>dt</i>)	3.36	H-31	1.87
H-17s (<i>dd</i>)	2.84	H-32 (very broad)	7.8
H-18a (<i>dd</i>)	3.21	H-33 (broad)	7.6
H-18s (ddd)	4.09	H-34 (broad)	7.5





$[(R_p, R, R_{Ru})-[Ru(\eta^6-p-cym)(QUIPHANEPROX)Cl]^+BPh_4 (8)$

$$[\alpha]_D^{20} = +221 \ (c = 0.069, CHCl_3)$$



Table S6. Chemical shift values assigned to the protons of complex (R_p, R, R_{Ru}) -8 in CDCl₃.

H-3 (s)	7.73	H-22t (<i>t</i>)	4.50
H-6 (d_{AB})	7.02	H-23 (ddd)	4.22
H-7 (d_{AB})	7.13	H-25 (<i>d</i>)	4.79
H-9a (<i>m</i>)	3.06	H-25' (<i>d</i>)	4.88
H-9s (<i>m</i>)	5.57	H-26 (<i>d</i>)	5.12
H-10a (<i>m</i>)	2.90	H-26' (<i>d</i>)	4.86
H-10s (<i>m</i>)	3.19	H-28 (<i>sept</i>)	2.00
H-12 (dd_{AB})	6.60	H-29 (<i>d</i>)	069
H-13 (dd_{AB})	6.71	H-29' (<i>d</i>)	0.88
H-15 $(dd)_{AB}$	5.50	H-31 (s)	1.18
H-16 $(dd)_{AB}$	5.45	H-32 (<i>sept d</i>)	2.37
H-17a (<i>dd</i>)	3.34	H-33 (<i>d</i>)	1.07
H-17s (<i>dt</i>)	2.79	H-33' (<i>d</i>)	0.90
H-18a (<i>m</i>)	3.15	BPh ₄ o (8 H)	7.38
H-18s (dd)	4.00	$BPh_4 m (t, 8 H)$	7.03
H-19 (s)	3.01	$BPh_4 p (t, 4 H)$	6.91
H-22c (<i>dd</i>)	4.65		



Figure S3. The section of the ¹H-NOESY diagram (400.13MHz, 293 K, CDCl₃) for complex (R_p ,R, R_{Ru})-8 showing the NOE correlation between the protons H-23 and the aromatic protons H-27 and H-28 of *p*-cymene ligand. A significant NOE correlation of the aromatic *o*- and *p*-protons of tetraphenylborate anion with H-23, H-22t (red circled) as well as with the aromatic protons of *p*-cymene ligand (bleu circled) is also noticeable.



$[(R_p, S, R_{Ru})-[Ru(\eta^6-p-cymene)(QUIPHANEPROX)Cl]^+BPh_4 (9)$

$$[\alpha]_{D}^{20} = +575 \ (c = 0.105, CHCl_3)$$



Table S7. Chemical shift values assigned to the protons of complex (R_p, S, R_{Ru}) -9.

H-3 (s)	7.59	H-22c (<i>dd</i>)	4.78
H-6 (d_{AB})	7.05	H-23 (ddd)	4.49
H-7 (d_{AB})	7.12	H-25 (broad s)	5.07
H-9a (<i>m</i>)	3.08	H-25'	n.d.
H-9s (<i>m</i>)	5.25	H-26 (<i>d</i>)	4.95
H-10a (<i>m</i>)	2.92	H-26'	n.d.
H-10s (<i>m</i>)	3.06	H-28 (very broad)	1.3?
H-12 (dd_{AB})	6.59	H-29 (very broad)	~0.1
H-13 (dd_{AB})	6.70	H-29' (very broad)	~0.4
H-15 (<i>dd</i>)	5.48	H-31 (broad)	1.60
H-16 (<i>dd</i>)	5.39	H-32 (broad)	2.32
H-17a (<i>dd</i>)	3.35	H-33 (<i>d</i>)	1.12
H-17s (<i>dd</i>)	2.79	H-33' (<i>d</i>)	0.99
H-18a (<i>dt</i>)	3.17	BPh ₄ o (8 H)	7.01
H- $\overline{18s}$ (dd)	3.96	$BPh_4 m (t, 8 H)$	7.4
H-19 (s)	2.91	$BPh_4 p (t, 4 H)$	6.90
H-22t (<i>d</i>)	4.79		



Figure S4. The section of the ¹H-NOESY diagram (400.13 MHz, 293 K,CDCl₃) of the complex (R_p , S, R_{Ru})-9 showing the NOE correlations between aromatic protons H-27 and H-28 of *p*-cymene and H-24 of the isopropyl group in the oxazoline ring. Significant NOE contacts of the *ortho-* and *para-* aromatic protons of tetraphenylborate anion with H-25, H-26 of the isopropyl group in the oxazoline ring is also noticeable (bleu circled).





$[(R_p, R_{Ru})-[Ru(\eta^6-p-cymene)(QUIPHANEDIMOX)Cl]^+BPh_4 (10)$

$$[\alpha]_{D}^{20} = +357 \ (c = 0.0.086, CHCl_3)$$



Table S8. Chemical shift values assigned to the protons of complex $[(R_p, R_{Ru})-10]$.

H-3 (s)	7.66	H-22c (d_{AB})	4.51
H-6 (d_{AB})	7.03	H-22t (d_{AB})	4.42
H-7 (d_{AB})	7.12	H-25 (bd)	5.10
H-9a (<i>dt</i>)	3.12	H-25'(<i>d</i>)	5.00
H-9s (<i>m</i>)	5.38	H-26 (very broad)	5.5
H-10a (<i>m</i>)	2.90	H-26'(very broad)	4.9
H-10s (<i>m</i>)	3.10	H-28 (broad)	2.26
H-12 (dd_{AB})	6.58	H-29 (very broad)	0.5
H-13 (dd_{AB})	6.70	H-29' (very broad)	-0.1?
H-15 (<i>dd</i>)	5.47	H-31	n.d.
H-16 (<i>dd</i>)	5.41	H-32 (<i>s</i>)	1.58
H-17a (<i>dd</i>)	3.35	H-33 (s)	1.38
H-17s (<i>dt</i>)	2.80	BPh ₄ o (8 H)	7.38
H-18a (<i>dt</i>)	3.18	$BPh_4 m (t, 8 H)$	7.00
H-18s (<i>dd</i>)	4.00	$BPh_4 p (t, 4 H)$	6.89
H-19 (s)	2.99		

Electronic Circular Dichroism Section



Figure S5. ECD spectrum (THF) of ligand (R_p, S) -2.



Figure S6. ECD spectrum (THF) of compound (R_p) -14.

Absorption and ECD spectra were recorded at room temperature on a JASCO J815 spectropolarimeter, using 0.1 mm cells and concentrations of about 1×10^{-3} M in tetrahydrofurane (THF). During the measurement, the instrument was thoroughly purged with nitrogen.

Theoretical Section

A preliminary search of the most stable conformations has been performed at the molecular mechanics (MM) level using Spartan02, profiling the strain energy for full rotations in turn of the *p*-cymene isopropyl group and *p*-cymene itself in **6-10** and the phenyl and isopropyl moieties at the oxazoline ring in **6-9**. Then, MM conformations have been optimized at the quantum mechanical (QM) density functional theory (DFT) level using the B97-D density functional in combination with the SV(P) basis set, as implemented within Gaussian 09. Solvent effects were not included. Chiroptical properties were calculated for the QM equilibrium geometries at the time-dependent density functional theory (TD-DFT) level, combining the B3LYP density functional with the SV(P) basis set. Rotational strengths were obtained for the first 100 electronic transitions.

A series of Tables follows with optimized QM geometries at B97-D/SV(P) level plus corresponding pictures of the complexes examined in the paper.

С	4.313832	0.911750	0.982575	H -2.765852	2.131827	-3.224328	
С	2.279236	-1.148668	0.950564	C -3.090742	1.701419	-1.076895	
С	3.033360	1.195002	0.373553	N 0.718333	0.431421	-0.059264	
С	4.392375	-0.223109	1.787561	N -1.800609	1.076981	-0.702387	
С	3.412059	-1.237039	1.751634	Ru -1.230238	-0.498428	0.499999	
С	1.974876	0.162284	0.421941	Cl -1.037179	-1.743467	-1.577241	
Н	5.330247	-0.430865	2.316983	C -2.111037	0.379785	2.349799	
н	3.646641	-2.199677	2.224011	C -1.691072	-2.431521	1.686078	
С	1.682395	-2.449059	0.444869	C -0.897574	-0.291459	2.679725	
н	0.608739	-2.376502	0.255060	C -3.112057	-0.386032	1.646550	
Н	1.840062	-3.214109	1.226946	C -2.897805	-1.739754	1.281287	
С	5.653201	1.542652	0.597625	C -0.712255	-1.688772	2.390474	
Н	6.398352	1.160720	1.317236	H -0.072109	0.267565	3.130476	
Н	5.680921	2.638444	0.693440	H -4.012949	0.117618	1.282531	
С	6.151912	1.143831	-0.866746	H -3.628074	-2.247262	0.643781	
н	7.248776	1.012823	-0.814513	H 0.241251	-2.158685	2.642122	
н	5.957451	1.979345	-1.564491	C -1.475332	-3.854973	1.263695	T
С	2.329793	-2.985420	-0.921296	H -0.508624	-4.244442	1.622410	
н	1.532665	-2.947938	-1.683359	H -1.498363	-3.910273	0.158024	
н	2.610384	-4.043044	-0.764603	H -2.289390	-4.493364	1.657813	
С	3.517580	-2.170832	-1.364845	C -2.344111	1.843271	2.667991	
С	5.454437	-0.103140	-1.362801	H -3.129681	2.196200	1.970733	
С	4.800350	-2.391156	-0.821045	C -1.092251	2.711172	2.452430	
С	3.310025	-0.997654	-2.116521	H -1.341568	3.778272	2.596656	
С	4.272460	0.020726	-2.119177	H -0.683749	2.573761	1.435714	
С	5.759506	-1.368211	-0.818386	H -0.297803	2.458075	3.179833	
н	5.008149	-3.331606	-0.293050	C -2.891972	1.976753	4.106075	
н	2.336870	-0.836991	-2.598842	H -3.128172	3.034054	4.328760	1
Н	4.045880	0.978216	-2.606352	H -2.138666	1.628316	4.838715	3.356
Н	6.706044	-1.512406	-0.280074	H -3.810587	1.376467	4.244654	
С	2.748524	2.414162	-0.333247	C -4.206996	0.739157	-1.412313	
С	1.525949	2.521718	-0.990945	C -6.312275	-1.035128	-2.011360	
н	1.277375	3.413492	-1.575188	C -5.458637	0.879027	-0.779160	
С	0.535342	1.546281	-0.799694	C -4.018849	-0.285600	-2.359929	
С	3.660497	3.616870	-0.381425	C -5.066937	-1.172470	-2.651343	
н	4.564989	3.424243	-0.985545	C -6.510293	-0.003950	-1.076577	
Н	3.991827	3.902346	0.632704	H -5.610032	1.687132	-0.049753	
н	3.135273	4.477554	-0.830081	H -3.043789	-0.414035	-2.841208	
С	-0.840562	1.784325	-1.214989	H -4.908039	-1.976854	-3.380053	
0	-1.188925	2.788163	-2.021311	H -7.481979	0.114532	-0.581488	
С	-2.631884	2.621242	-2.241918	H -7.129585	-1.728912	-2.244620	
Н	-3.097137	3.619237	-2.239634	H -3.406338	2.317523	-0.209102	

Table S9. Structure and Cartesian coordinates of (R_{p}, R, R_{M}) -**6a**.

С	-4.321705	1.260018	0.566122	н	2.552877	-3.181313	2.945357	
С	-2.263754	0.729756	-1.372055	С	2.868000	-1.264824	1.829284	
С	-3.112966	0.593842	0.993055	Ν	-0.848067	-0.175459	0.345049	
С	-4.304238	1.873783	-0.687524	Ν	1.629024	-0.736692	1.232648	
С	-3.311778	1.592327	-1.653831	Ru	1.297410	0.700025	-0.221950	
С	-2.045171	0.391006	0.007464	CI	0.575624	2.113131	1.627361	
н	-5.189452	2.437652	-1.006595	С	2.820647	2.270213	-0.627270	
н	-3.478406	1.917305	-2.688880	С	1.855637	0.239231	-2.465461	
С	-1.597060	-0.066782	-2.464667	С	1.684583	2.526924	-1.481913	
н	-0.604863	-0.376646	-2.118990	С	3.421650	0.978722	-0.693877	
н	-1.475384	0.563968	-3.363373	С	2.950832	-0.021640	-1.604689	
С	-5.699424	1.089665	1.203035	С	1.201338	1.524189	-2.351079	
н	-6.375599	1.800296	0.696227	н	1.145831	3.474095	-1.381787	
н	-5.736501	1.349234	2.271853	н	4.234122	0.729929	-0.009017	
С	-6.312146	-0.375905	1.014793	н	3.422558	-1.008231	-1.613729	
н	-7.396115	-0.257525	0.830588	н	0.302986	1.719469	-2.941531	T
н	-6.203354	-0.945590	1.956126	С	1.461543	-0.791370	-3.491981	
С	-2.398860	-1.393923	-2.897196	н	0.522371	-0.534580	-4.004942	
н	-1.705408	-2.249677	-2.799781	н	1.361834	-1.791735	-3.032519	
н	-2.662730	-1.299991	-3.966277	н	2.262319	-0.856433	-4.255263	
С	-3.641554	-1.6212Ru	-2.069656	С	3.348786	3.359597	0.279909	
С	-5.627775	-1.121693	-0.109810	н	2.470232	3.948432	0.600804	
С	-4.859130	-1.002322	-2.422929	С	4.282323	4.265995	-0.557071	
С	-3.547803	-2.206553	-0.791842	н	5.168697	3.699884	-0.903808	
С	-4.532673	-1.961399	0.174878	н	4.632736	5.112733	0.061952	
С	-5.842198	-0.755390	-1.454622	н	3.764885	4.675855	-1.444957	
н	-4.984863	-0.600080	-3.437043	С	4.047642	2.835171	1.543055	
н	-2.636827	-2.752210	-0.511578	н	4.321055	3.684891	2.194130	Y
н	-4.382502	-2.318467	1.201942	н	4.983657	2.295114	1.298075	
н	-6.725318	-0.158516	-1.718838	н	3.367542	2.171431	2.106445	
С	-2.909691	0.042933	2.305938	н	3.467411	-0.411257	2.196207	/
С	-1.754159	-0.700359	2.533640	С	3.679381	-2.057270	0.821818	1
н	-1.562593	-1.151576	3.512479	С	5.144992	-3.465005	-1.132089	
С	-0.737037	-0.734670	1.563778	С	5.041143	-1.773837	0.615647	
С	-3.834864	0.260552	3.478276	С	3.058683	-3.067305	0.058435	
н	-4.791261	-0.278667	3.354151	С	3.786547	-3.766939	-0.915977	
н	-4.069458	1.333254	3.597519	С	5.773586	-2.472897	-0.360203	
н	-3.364883	-0.097830	4.410288	н	5.528947	-0.995010	1.217435	
С	0.609262	-1.173506	1.909114	н	1.994616	-3.289052	0.213126	
ο	0.857597	-1.970366	2.945815	н	3.296510	-4.548467	-1.510030	
С	2.311938	-2.107816	3.029839	н	6.834514	-2.242748	-0.517491	
н	2.629562	-1.722477	4.013679	Н	5.713979	-4.009461	-1.895722	

Table S10. Structure and Cartesian coordinates of (R_p, R, S_M) -6a.

C 4.05475 0.416230 1.397786 H - 2.72966 3.37986 -2.879756 C 2.194526 1.46230 3.20013 C - 300787 1.52955 -1.551366 C 2.829233 0.91974 0.814706 H - 3.043973 1.004389 -2.488113 C 4.13107 0.954357 1.64344 C - 4.290613 1.397503 -0.774931 C 3.24076 1.47376 1.04636 C - 6.61229 0.8292476 0.741272 C 1.856242 -0.061565 0.288558 C - 5.315789 0.58238 -1.297066 H 3.046001 - 2.940728 1.079548 C - 5.594564 1.71374 1.263393 C 1.716315 -2.402556 -0.860220 C - 6.475177 0.33634 -0.542345 H 0.628802 -2.381223 -1.005908 H - 5.193372 0.140617 -2.291675 H 1.979724 3.428128 0.557464 H - 3.640133 2.593764 0.920541 H 0.628802 -2.381223 -1.005908 H - 7.270134 2.155459 2.261754 H 5.318149 2.127142 2.032664 H -7.270139 0.925735 C 5.37689 J 1.81085 1.474366 H - 7.270139 0.256735 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187224 H 5.318149 2.127142 2.032664 H -7.270139 0.955190 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187224 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 H 5.384251 2.542049 0.21582 R U -1.21159 0.75703 -0.095190 C 2.35777 2.092381 -2.21795 C C -1.194882 -1.216375 -2474614 H 7.51487 -1.1616108 -2.00716 C C -0.05264 2.340206 1.386811 H 2.50743 -0.06312 -1.00767 C C -2.85748 -2.356128 0.215296 C 3.45541 0.199106 -2.365527 C C -3.215879 -1.193754 0.952492 C 3.45541 0.199106 -2.365527 C C -3.215879 -1.193754 0.952492 C 3.45141 0.199106 -2.365527 C C -3.215879 -1.193754 0.952492 C 3.45141 0.199106 -2.36527 C C -3.215879 -1.193754 0.952492 C 3.45141 0.199106 -2.36527 C C -3.75618 0.454888 C 4.39465 1.088458 -1.779382 H - 3.215875 -3.77218 0.153266 H 2.500451 0.884583 -2.797382 H - 3.215879 -3.055266 C 3.305459 -1.084683 -3.05129 - 0.751618 -2.448843 -0.821793 H 3.520615 0.58458 -3.05714 H -3.214978 -3.075264 2.07909 C 3.34244 3.433100 1.24074 C -0.15724 -2.290704 3.05589 C 3.37424 -3.43818 -3.306169 0.751961 H -4.215227 -3.772149 -0.365899 C 3.30429 -3.34248 -3.383101 -2.49074 C -0.15724 -3.277424 -4.345804 H 1.1643 -3.707618 -2.15607 C -0.010202 -0.351207 -3.056899									
C 2.19426 1.462803 0.230013 C 3.007807 1.592955 1.551366 C 2.832928 0.019974 0.814706 H 3.004397 1.004389 2.488113 C 4.131907 0.954357 1.643434 C 4.200613 1.397503 0.774931 C 3.240760 1.473766 1.046368 C - 6.612429 0.892476 0.741272 C 1.85624 0.061656 0.28558 C - 5.51758 0.555790 H 5.024084 1.351446 2.143248 C - 4.441068 1.967302 0.505790 H 5.024084 2.381223 -1.005908 H - 5.193872 0.140617 - 2.291675 H 0.628002 - 2.381223 -1.005908 H - 5.703944 2.155459 2.261754 H 0.628042 0.43203 2.036513 H - 7.270129 - 0.279735 - 0.055498 H 5.318149 2.127142 2.032694 H - 7.514532 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 5.318149 2.127142 2.032694 H - 7.514532 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 5.348147 1.1616108 -2.904706 C - 1.012686 -1.132924 2.103521 H 2.60736 -3.065580 -2.753824 C - 2.306552 - 0.582754 1.884223 C 3.36677 - 1.191688 -2.021712 C - 0.66544 2 - 2340206 1.368611 C 5.425633 0.608312 1.004073 C - 3.215879 4.1502542 C - 3.265873 - 1.191638 - 2.030712 C - 0.66544 2 - 2340206 1.368611 C 5.472897 - 1.662563 -1.67482 C - 3.256128 0.454888 H - 1.215325 - 0.775125 - 0.582740 1.382420 C - 3.45141 0.199166 - 2.365127 C - 1.548167 -225618 0.454888 H - 1.215325 - 0.775125 - 0.582749 1.502542 C - 3.776215 - 1.092381 H - 4.178626 - 0.716488 0.755326 H - 4.504937 -2.744391 - 1.603213 H + 4.178626 - 0.716488 0.755326 H - 4.504937 -2.744391 - 1.603213 H + 4.128317 - 3.472247 1.502542 C - 3.776218 -0.236520 C - 0.517209 C - 0.517240 - 0.378264 -0.775094 C - 3.707618 -0.236520 C - 0.517240 - 0.573264 H - 1.164379 -0.571961 H + 3.214978 - 3.075266 + 0.775094 C - 3.707618 -0.236520 C - 0.517240 - 0.378214 - 0.48804 H 1.116436 3.707618 -0.246008 H + 4.128437 - 3.472679 C - 3.766102 -2.468079 N -4.349183 - 0.221704 -4	С	4.056475	0.416280	1.397786	н	-2.729669	3.379896	-2.879756	
C 2.829283 0.910974 0.814706 H - 3.043973 1.004389 2.488113 C 3.13107 0.959435 1.643434 C - 4.290613 1.397503 -0.774931 C 3.240760 -1.873766 1.046368 C - 6.612429 0.892476 0.741272 C 1.86124 -0.061556 0.288558 C - 5.31579 0.588238 -1.297066 H 3.049601 -2.940728 1.079548 C -5.594564 1.713744 1.263393 C 1.716315 -2402556 0.860220 C - 6.475177 0.336364 -0.5424345 H 0.628802 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 H 1.997324 -3.428128 -0.557464 H -3.640133 2.533764 0.920541 C 5.376699 1.181085 1.473466 H -5.703944 2.155459 2.261754 H 5.318149 -2.17424 2.032564 H -3.640133 2.533764 0.920541 C 5.376599 1.181085 1.473466 H -7.70129 -0.296735 -0.955498 H 5.318149 -2.17424 2.032564 H -7.751452 0.059318 1.3325959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 H 5.384251 2.542049 0.215882 Ru -1.291159 0.757903 -0.095190 C 2.357577 -2.092381 .2.291795 C -1.194882 -1.216375 -2.474614 1.573417 -1.616108 -2.904776 C -0.665442 -2.340206 1.386811 C 5.425630 .063312 -1.046673 C -2.305527 -0.352548 H 2.504736 -3.065580 -2.753824 K -2.325518 0.451296 C 3.45547 -1191688 -2.200712 C -0.665442 -2.340206 1.386811 C 4.339465 1.088455 -1.79382 H 0.348437 -2.742247 1.502542 C 4.78879 -1.662563 -1.674382 C -3.215879 -1.337579 -2.362400 H 4.964987 -2.74391 -1.602213 H +2.15235 -3.77218 0.153266 H 2.504745 0.554548 -2.338154 H -1.215325 -3.77218 0.153266 H 2.500451 0.584548 -2.338154 H +1.215325 -3.77218 0.153266 H 4.142279 -2.074215 1.09503 H + 4.178626 0.3755326 H 2.52349 -2.308256 0.664808 H +4.639628 -2.795424 -0.486804 H 4.142479 -3.0751961 H +3.214978 -3.075264 1.772095 C 3.342541 0.585488 -2.338154 H +4.124317 -3.94242 -0.486804 H 1.116437 -0.571961 H +4.242317 -3.94242 -0.486804 H 1.116437 -0.571961 H +4.242317 -3.94242 -0.486804 H 1.116437 -0.571961 H +4.242317 -3.94242 -0.486804 H 1.116437 -3.075194 -0.156292 H +0.632962 -0.351047 -3.057999 C 3.34244 -3.433100 1.249074 C -0.157241 -5.37111 H 3.550615 -3.25638 2.3193	С	2.194526	-1.462803	0.230013	С	-3.007867	1.592955	-1.551366	
C 4.131007 - 0.954357 1.643434 C 4.290613 1.397503 -0.774931 C 3.240760 - 1.837366 1.046368 C 6.612429 0.89276 0.741272 C 1.856242 -0.061656 0.288588 C -5.315789 0.588238 -1.297066 H 5.024084 -1.351446 2.143248 C -4.441068 1.967302 0.505790 H 5.024084 -1.351446 2.143248 C -4.441068 1.967302 0.505790 C 1.716315 -240255 -0.360220 C -6.475177 0.336346 -0.542345 H 0.628802 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 H 1.997324 -3.428128 -0.55746 H -5.703944 2.155459 2.261754 H 0.628802 -0.381223 -1.0053613 H -7.514352 0.693918 1.332959 C 6.029561 1.476481 0.04136 N 0.639743 0.35749 0.218724 H 5.38149 2.127142 2.032694 H -7.514532 0.693918 1.332959 C 6.029561 1.476481 0.04136 N 0.639743 0.305749 0.187924 H 7.118648 1.312389 0.140178 N 1.828146 1.112004 -0.808468 H 5.884251 2.542049 -0.215882 Ru -1.291159 -0.757903 0.095190 C 2.3356777 -2092381 2.201795 C -1.012666 -1.129542 2.103521 C 3.45671 -1.01618 -2.004702 C -0.665442 2.340266 1.386811 C 5.425633 0.605381 -2.753824 C -2.857484 8.236128 0.215296 C 3.366772 -1.91688 2.200712 C -0.665442 -2.340266 1.386811 C 5.4788979 -1.662563 1.647438 C C -3.215879 -1.139754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 H 4.946987 -2.744391 -1.603213 H 4.178262 -0.716458 0.755326 C 3.764712 -0.05503 H -2.592760 1.377218 -0.152492 C 3.445141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 4.3964987 -2.744391 -1.603213 H 4.125825 -0.37579 2.3652400 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 4.324049 3.438100 1.249074 C -0.157834 1.331207 H 6.58640 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 3.23429 3.438100 1.249074 C -0.157834 1.231207 3.065899 C 3.70618 -2.236522 0.587044 2.317311 H 4.1542179 2.168073 -1.829338 C H -4.124317 -3.94244 -0.468604 H 1.11436 3.707618 -0.036611 H -4.12337 -3.075264 1.772095 C 3.23429 3.438100 1.249074 C -0.157834 1.331217 H 3.550615 3.256538 2.319312 H -0.041222 -3.23744 2.345629 C 3.432494 3	С	2.829283	0.910974	0.814706	н	-3.043973	1.004389	-2.488113	
C 3.240760 -1.873766 1.046368 C -6.61242 0.892476 0.741272 C 1.856242 0.061656 0.288558 C -5.59456 1.71374 1.263393 C -5.594564 1.713741 1.263393 C -5.594564 1.713744 1.263393 C -6.4441068 1.967302 0.505790 H 3.496001 -2.940728 1.079548 C -5.594564 1.713744 1.263393 C 1.716315 -2402556 0.366020 C -6.475177 0.336346 -0.542435 H 6.628802 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 H 1.997324 -3.428128 0.557464 H -3.640133 2.593764 0.920541 C 5.376689 1.181085 1.473466 H -7.570394 2.251754 H 6.080484 0.543303 2.036513 H -7.7514532 0.955498 H 5.318149 2.127142 2.032694 H -7.514532 0.695318 1.332959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312289 0.140178 N -1.828146 1.112004 -0.808468 H 5.884251 2.542049 0.215882 Ru 1.291159 0.757903 0.095190 C 2.357577 -2.092381 -2.291795 CI -1.19482 -1.216375 -2.474614 I .577417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 C 3.45633 0.608312 -1.040673 C -3.205512 0.535182 0.458184 C -3.206721 C 0.665432 -1.074822 C -3.215279 C 3.45633 0.608312 -1.040673 C -3.206526 0.357579 2.362400 H 4.964987 -2.744391 -1.60223 H -2.592760 0.337579 2.362400 H 4.964987 -2.744391 -1.60223 H -2.592760 0.337579 2.362400 H 4.954987 -2.744391 -1.603213 H -4.215325 -3.77218 -0.153266 C .337657 -1.693584 C .3216597 C -1.548167 -2.925618 0.454888 C .3706173 -1.69379 0.571961 H -3.214978 -3.075266 -1.772095 C .542563 0.668488 H -4.639628 -2.99542 -0.997493 H 4.598497 -2.744391 -1.603213 H -4.125325 -3.77218 -0.153266 C .3706477 -2.74125 -1.095003 H -4.213427 -3.052642 C .3706477 -2.694868 -3.040826 H 0.993007 -0.775694 2.670099 C .342494 3.433100 1.249074 C -0.15784 -1.23127 -3.053266 C .447075 1.663588 -0.404826 H 0.993007 -0.775694 2.670099 C .342494 3.433100 1.249074 C -0.15784 -1.231207 3.05589 C .370472 -1.69378 -1.055602 C -0.010202 -0.35714 -5.3711 H -3.550615 3.256518 2.319312 H -0.041222 -2.327442 -345822 H 2.803748 4.393105 1.157481 H -1.162360 -1.0728900 4.872791 C .0447075 1.663588 -0.404826 H 0.993007 -0.775694 2.6	С	4.131907	-0.954357	1.643434	С	-4.290613	1.397503	-0.774931	
C 1.85242 0.061656 0.288558 C -3.315789 0.588238 1.297066 H 3.496001 -2.940728 1.079548 C -4.441068 1.967302 0.505790 H 3.496001 -2.940728 1.079548 C -5.594564 1.713744 1.263393 C 1.716315 -2.402556 0.860220 C -6.475177 0.336346 -0.542345 H 0.628802 -2.381223 1.00598 H -5.193872 0.140617 -2.291675 H 0.628802 -2.381223 1.005981 H -7.270129 0.296735 -0.955498 H 5.318149 2.127142 2.032694 H -7.514532 0.693918 1.332959 K 0.608404 0.543303 2.036513 H -7.270129 0.296735 -0.955498 H 5.318149 2.127142 2.032694 H -7.514532 0.693918 1.332959 K 0.608404 0.14768 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 K 0.5884251 2.542049 -0.215882 Ku -1.291159 -0.75903 -0.095190 C 2.357577 -2.092381 -2.201752 C -0.665442 -2.340266 1.386811 C 5.425633 0.608312 -0.04673 C -2.306552 -0.582754 1.884223 C 3.566772 -1.191688 -2.20712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -0.04673 C -2.306552 -0.582754 1.884223 C 3.4339465 0.688455 -1.797382 H 0.344837 -2.742247 1.502542 C 3.4339465 0.688455 -1.797382 H 0.344837 -2.742247 1.502542 C 3.740727 -0.62534 -0.674382 C -3.215879 -0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.142179 2.168073 -1.829388 H + -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.142179 2.168073 -1.829388 C -3.766110 -2.984843 -0.821793 H 6.586410 -1.168379 -0.57161 H -3.219873 -0.51207 0.56589 C 2.523482 -2.308256 0.64648 H +0.393007 -0.775094 2.670099 C 3.24249 3.433100 1.24907 C -0.157242 -0.351207 -3.65689 C 1.370887 2.657984 -0.035617 H -4.2329542 -0.397433 H 3.540649 3.79617 H -4.639668 -1.72095 C 3.44249 3.433100 1.24907 C -0.157824 -0.366894 H 4.314049 3.540169 0.735017 H -4.63266 -3.77718 H 3.51469 -3.70518 -0.75157 H -0.612229 -0.851797 3.82711 H 3.51655 3.25638 2.319312 H -0.041282 -3.227424 2.345822 H 2.803748 4.391325 1.152081 H -0.012249 0.4877791 C -0.47775 1.669368 -0.404826 H -0.993007 -0.775094 2.670099 C 3.44249 3.433100 1.249074 C -0	С	3.240760	-1.873766	1.046368	С	-6.612429	0.892476	0.741272	
H 5.024084 -1.351446 2.143248 C -4.441068 1.967302 0.505700 H 3.496001 -2.940728 1.079548 C -5.59456 1.71374 1.263393 C -5.69456 1.71615 -2.402556 -0.860220 C -6.475177 0.36346 -0.542345 H 0.628802 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 H 3.08208 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 C 5.376899 1.181085 1.473466 H -5.703944 2.155459 2.261754 H 6.080444 0.533303 2.036513 H -7.270129 -0.296735 -0.955498 H 7.118648 1.312389 0.140178 N -6.893918 1.323259 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112049 -0.080468 H 5.384251 2.542049 0.215882 Ru -1.291159 0.757903 -0.095190 C 2.357577 -2.092381 -2.291795 C -1.194882 -1.216375 -2.474614 H 1.578417 -1.616108 -2.004706 C -1.012686 -1.132924 2.103521 H 2.500743 -3.065580 -2.753824 C -2.85748 -2.356128 0.215296 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 H 2.504745 0.068312 -1040673 C -3.205527 -0.582754 1.884223 C 4.788979 -1.662563 -1.674382 C -3.215879 -1.133754 0.952492 C 3.415141 0.199106 -2.365127 C -3.205527 -2.742247 1.502542 C 4.339465 1.088455 -1.674382 C -3.215879 -1.193754 0.952492 C 4.339465 1.088455 -1.674382 C -3.215879 -2.326240 H 4.964987 -2.744391 -1.603213 H -2.92760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -2.15225 -3.772718 -0.153266 H 4.12179 2.168073 -1.229338 C -3.766110 -2.948843 -0.821793 H 4.536410 -0.55438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.586410 -0.55438 -0.404628 H -3.219828 -0.97493 C 1.370887 2.657848 -0.035511 H -4.124317 -3.942424 -0.486804 H 4.116435 -0.751661 H -4.539628 -2.295422 -0.97493 C 1.370887 2.657848 -0.035611 H +4.52381 -3.075266 -1.772055 C 2.523489 2.308256 0.664808 H + 4.639628 -2.295422 -0.97493 C 1.370887 2.657848 -0.035617 H +4.124317 -3.942424 -0.486804 H 4.314044 3.540169 0.735617 H H -0.612229 0.857104 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -3.237424 2.345822 H 2.803748 4.391325 1.152081 H +0.061229 0.857104 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -3.237424 2.345822 H 2.8037	С	1.856242	-0.061656	0.288558	С	-5.315789	0.588238	-1.297066	
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C 1.716315 -2.402556 -0.860220 C -6.475177 0.336346 -0.542345 H 0.62802 -2.381223 -1.005908 H -5.193872 0.140617 -2.291675 H 1.987324 -3.422128 -0.557464 H -5.073944 2.155459 2.261754 H 6.080484 0.543303 2.035513 H -7.270129 -0.296735 -0.955498 H 5.318149 2.127142 2.032694 H -5.739344 2.155459 2.261754 H 5.3025561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 H 7.118648 1.312389 0.215882 Ru 1.291159 -0.75793 0.095190 C 2.357577 -2.092381 -2.291795 Cl -1.194882 -1.216375 -2.474614 H 2.573417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 C 3.566772 -1.191688 -2.20712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608122 -1.040673 C -2.306552 -0.582754 1.884223 C 3.45673 0.608122 -1.040673 C -2.306552 -0.582754 1.884223 C 3.4515141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 H -3.259276 0.035757 -2.032384 H -2.592760 0.35757 2.362400 H 4.964987 -2.744391 -1.695203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.69203 H -4.178626 -0.716458 0.755326 H 2.500451 0.58448 -2.833828 H +1.215325 -3.772718 -0.153266 C 1.370887 -0.774125 -1.095203 H + 3.214978 -3.075266 -1.772095 H 4.412179 -2.657934 -0.035117 H +3.214978 -3.075266 -1.772095 C 2.522489 2.308256 0.664808 H +4.639628 -2.298542 -0.997493 H 6.586410 -1.168379 -0.571961 H +3.214978 -3.075266 -1.772095 C 1.370887 -2.657984 -0.035611 H +4.124317 -3.94244 -0.486804 H 4.142179 -2.657934 -0.035611 H +4.124317 -3.94244 -0.486804 H 4.142179 -2.657934 -0.035611 H +4.124317 -3.94244 -0.486804 H 4.314404 -3.540169 0.735017 H 0.612229 -0.85714 5.137311 H 3.510615 -3.256538 2.319312 H -0.041282 -2.327442 -4.345822 H 2.80748 -3.434806 H 0.993007 -0.775094 2.670099 C 0.342494 +3.43100 -1.52081 H +0.612229 -0.85714 5.137311 H 3.510615 -3.256538 2.319312 H -0.041282 -2.327442 -3.45822 H 2.80748 -3.434204 -1.50280 C -0.115421 0.995128 3.200445 D -1.175897 -3.446402 -1.503496 H 0.715714 -0.292484 -0.86934 D -1.175897 -3.446402 -1.503496 H 0.71521	н	3.496001	-2.940728	1.079548	С	-5.594564	1.713744	1.263393	
H 0.628802 -2.381223 -1.005908 H -5.193872 0.10617 -2.291675 H 1.997324 -3.428128 -0.557464 H -3.640133 2.593764 0.920541 C 5.376899 1.81085 1.873466 H -5.703944 2.155459 2.261754 H 5.318149 2.127142 2.032694 H -7.514532 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.183724 0.095190 C 2.357577 -2.092381 -2.291795 C -1.194882 -1.216375 2.474614 V 2.607436 -3.065580 -2.753824 C -2.367574 2.035211 C 5.366777 -1.914882 -1.219159 -0.575930 0.095190 C 5.366777 -1.91688 -2.00712 C -0.665442 -2.340206 1.386811 C 5.36777 -1.09288 -2.00712 C -1.548167 -2.925618 0.454888 C 3.39465 1.088455 -1.704382 C -3.2158	С	1.716315	-2.402556	-0.860220	С	-6.475177	0.336346	-0.542345	
H 1.997324 -3.428128 -0.55764 H - 3.640133 2.593764 0.920541 C 5.376899 1.181085 1.473466 H - 5.703944 2.155459 2.261754 H 6.080484 0.543303 2.036513 H - 7.770129 -0.26735 -0.955498 H 5.318149 2.127142 2.032694 H - 7.514532 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828144 1.11204 -0.808488 H 5.584251 2.542049 -0.215882 Ru -1.291159 -0.757903 -0.095190 C 2.357577 -2.092381 -2.291795 C 1 -1.194882 -1.21637 -2.474614 H 2.507436 -3.065580 -2.753824 C 1 -0.10268 -1.132924 2.103521 H 2.507436 -3.065580 -2.753824 C 2 -2.85748 -2.356128 0.215296 C 3.526577 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -1.040673 C -3.205512 -0.482748 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 H 2.500451 0.585488 -2.833854 H -1.215325 -3.772718 -0.153266 H 2.500451 0.585488 -2.833854 H -1.215325 -3.772718 -0.153266 H 2.400457 -2.744391 -1.603213 H -4.124317 -3.942424 -0.486804 C 3.324978 -2.57984 0.035611 H -4.124317 -3.942242 -0.486804 C 3.34249 -1.63837 -0.571661 H + 4.63628 -2.298542 -0.997493 C 3.42494 -3.43010 -1.163379 -0.571061 H + 4.124317 -3.942242 -0.486804 C 1.116436 3.707618 -0.215602 C -0.157384 -1.231127 4.437158 H 4.31404 3.540169 0.735017 H +0.61229 -0.85704 2.670099 C 0.447075 1.669388 -0.404826 H 0.993007 -0.775094 2.670099 C 0.447075 1.669388 -0.404826 H 0.993007 -0.757094 2.670099 C 0.447075 1.66938 -0.404826 H 0.993007 -0.757094 2.670099 C 0.432429 4.333100 1.429074 C -0.157834 -1.231217 4.437158 H 2.80374 4.331325 1.152081 H + 0.41282 -232742 4.345822 H 2.80374 4.331325 1.152081 H +0.041282 -232742 4.345822 H 2.80374 4.331302 1.152081 H + 0.041282 -327442 4.345822 H 2.80374 4.331302 1.152081	н	0.628802	-2.381223	-1.005908	н	-5.193872	0.140617	-2.291675	
C 5.376899 1.181085 1.473466 H -5.703944 2.155459 2.261754 H 6.080484 0.543303 2.036513 H -7.270129 -0.296735 0.955498 H 5.381349 2.127142 2.032694 H -7.51452 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N 1.828146 1.112004 -0.808468 C 2.357577 -2.092381 -2.291795 C 1 -1.194882 -1.216375 -2.474614 C 2.357577 -2.092381 -2.291795 C 1 -1.194882 -1.216375 -2.474614 A 1.573417 -1.616108 -2.904706 C -1.012666 -1.132924 2.03521 A 1.573417 -1.616108 -2.904706 C -1.012666 -1.132924 2.03521 C 3.566772 -1.191688 -2.200712 C -0.665444 -2.340206 1.386811 C 3.566772 -1.191688 -2.20712 C -0.665444 -2.340206 1.386811 C 3.451541 0.199106 -2.365127 C -3.251529 0.52754 1.884223 C 4.788979 -1.662563 -1.674382 C -3.215879 -1.193754 0.952492 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.3964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.3464987 -0.571961 H -3.214978 -3.075266 -1.72095 C 3.526470 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 3.524872 2.308754 0.664808 H -4.639628 -2.298542 -0.997493 H 6.586410 -1.168379 -0.571961 H -4.124317 -3.94244 -0.486804 H 1.116433 -307618 -0.215602 C -0.01020 -0.57107 -3.065899 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 -4.437158 H 3.350615 3.256588 2.319312 H -0.041282 -2.327422 -4.345822 H 3.34249 3.433100 1.249074 C -0.157834 -1.231217 -4.437158 H 3.350615 3.256588 2.319312 H -0.041282 -2.32742 -4.345822 H 3.34249 3.433100 1.249074 C -0.157834 -1.231217 -4.37158 H 3.350615 3.25658 2.319312 H -0.041282 -2.32742 -4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 -4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H -0.71264 1.37197 3.827711	н	1.997324	-3.428128	-0.557464	н	-3.640133	2.593764	0.920541	
H 6.080484 0.543303 2.036513 H -7.270129 -0.296735 -0.955498 H 5.18149 2.127142 2.032694 H -7.514532 0.693918 1.332959 C 6.029561 1.476481 0.041306 N 0.639749 0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 C 2.357577 2.092381 -2.219755 C -1.194682 -1.216375 2.474614 1 1.573417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -0.40673 C -2.305552 -0.582754 1.884223 C 3.34645 1.088455 1.793824 H -3.215879 1.192542 0.997493 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 C 5.704723 0.7741	С	5.376899	1.181085	1.473466	н	-5.703944	2.155459	2.261754	
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C 6.029561 1.476481 0.041306 N 0.639743 0.350749 -0.187924 H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 K - 1.32384 2.542049 -0.215882 Ru -1.291159 -0.757903 -0.095190 C 2.357577 -2.092381 -2.291795 C I -1.194882 -1.216375 -2.474614 H 1.573417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -1.040673 C -2.306552 -0.582754 1.884223 C 4.788979 -1.662563 -1.67482 C -3.215879 -1.193754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.79782 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.588438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.76510 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486849 H 1.11643 7.707618 -0.215602 C -0.01022 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.77504 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 3.530615 3.256538 2.319312 H -0.01220 -0.857014 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 3.530615 3.256538 2.319312 H -0.012482 -3.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.71261 1.371997 3.827711 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445	н	5.318149	2.127142	2.032694	н	-7.514532	0.693918	1.332959	
H 7.118648 1.312389 0.140178 N -1.828146 1.112004 -0.808468 H 5.884251 2.542049 -0.215882 Ru -1.291159 -0.757903 -0.095190 C 2.357577 -2.092381 -2.291795 C -1.194882 -1.216375 -2.474614 H 1.57347 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 H 2.607436 -3.065580 -2.753824 C -2.857448 -2.356128 0.215296 C 3.566772 -1.191688 -2.20712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -1.040673 C -3.215879 -1.133754 0.952492 C 3.415141 0.199106 -2.365127 C -3.215879 -1.133754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 0.774125 -1.05203 H -2.592760 0.357757 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 0.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H -3.152261 3.256538 2.319312 H -0.012820 -3.272742 4.3435822 H 2.803748 4.391325 1.152081 H -1.154320 -0.22900 4.872791 C -0.487075 1.669368 2.199071 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445	С	6.029561	1.476481	0.041306	Ν	0.639743	0.350749	-0.187924	(many many)
H 5.884251 2.542049 -0.215882 C 2.357577 -2.092381 -2.291795 C 1 -1.194882 -1.216375 -2.474614 H 1.573417 -1.616108 -2.904706 C -0.1012686 -1.13292 -2.103521 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425563 0.608312 -1.040673 C -2.305552 -0.582754 1.884223 C 3.451514 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 4.102179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116463 -370718 -0.215602 C -0.157834 -1.231207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C -0.157834 -1.231217 4.437158 H -3.14040 3.540169 0.735017 H 0.612229 -0.857014 5.137511 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.07774 -1.827324 H -1.062366 1.292811 3.690340	н	7.118648	1.312389	0.140178	Ν	-1.828146	1.112004	-0.808468	
C 2.357577 -2.092381 -2.291795 Cl -1.194882 -1.216375 -2.474614 H 1.573417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 H 2.607436 -3.065580 -2.753824 C -2.857448 -2.356128 0.215296 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -1.040673 C -2.306552 -0.582754 1.884223 C 4.788979 -1.662563 -1.674382 C -3.215879 -1.193754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.31404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327424 4.348522 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 H 1.116437 -1.503496 H 0.716214 1.377197 3.82714	н	5.884251	2.542049	-0.215882	Ru	-1.291159	-0.757903	-0.095190	
H 1.573417 -1.616108 -2.904706 C -1.012686 -1.132924 2.103521 H 2.607436 -3.065580 -2.753824 C -2.857448 -2.356128 0.215296 C 3.566772 -1.191688 -2.200712 C -0.665442 -2.340206 1.386811 C 5.425633 0.608312 -1.040673 C -2.306552 -0.582754 1.884223 C 4.788979 -1.662563 -1.674382 C -3.215879 -1.193754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.356111 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.42494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314204 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.266538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 H 1.715897 3.146402 -1.503496 H 0.712614 1.377197 3.827711 C -0.881059 1.390717 -0.912390 C -0.115421 0.395128 3.200445 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.390717 -0.912390 C -0.115421 0.395128 3.200445 H 2.803748 4.391325 1.152081 H 0.712614 1.377197 3.827711 C -0.881059 1.390717 -0.912390 C -0.115421 0.395128 3.200445 H 2.803748 4.391325 1.152081 H 0.712614 1.377197 3.827711 C -0.881059 1.390717 -0.912390 C -0.115421 0.395128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.37197 3.827711 C -2.607907 3.077724 -1.827324 H 1.062366 1.292811 3.69340	с	2.357577	-2.092381	-2.291795	CI	-1.194882	-1.216375	-2.474614	
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C 5.425633 0.608312 -1.040673 C -2.306552 -0.582754 1.884223 C 4.788979 -1.662563 -1.674382 C -3.215879 -1.193754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.83854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.94242 -0.486804 H 1.116436 3.707618 -0.21502 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.33125 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115241 0.995128 3.20445 D -1.175897 3.16402 -1.503496 H 0.712614 1.371997 3.827711 C -0.881059 1.990717 -0.912390 C -0.115214 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062249 (-0.895140)	с	3.566772	-1.191688	-2.200712	с	-0.665442	-2.340206	1.386811	
C 4.788979 -1.662563 -1.674382 C -3.215879 -1.193754 0.952492 C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.811059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445	с	5.425633	0.608312	-1.040673	с	-2.306552	-0.582754	1.884223	
C 3.415141 0.199106 -2.365127 C -1.548167 -2.925618 0.454888 C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	4.788979	-1.662563	-1.674382	с	-3.215879	-1.193754	0.952492	
C 4.339465 1.088455 -1.797382 H 0.344837 -2.742247 1.502542 C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.35611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	3.415141	0.199106	-2.365127	с	-1.548167	-2.925618	0.454888	
C 5.704723 -0.774125 -1.095203 H -2.592760 0.357579 2.362400 H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 C 3.766110 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	4.339465	1.088455	-1.797382	н	0.344837	-2.742247	1.502542	
H 4.964987 -2.744391 -1.603213 H -4.178626 -0.716458 0.755326 H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H	с	5.704723	-0.774125	-1.095203	н	-2.592760	0.357579	2.362400	
H 2.500451 0.585438 -2.833854 H -1.215325 -3.772718 -0.153266 H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314040 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.250615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H <t< td=""><td>н</td><td>4.964987</td><td>-2.744391</td><td>-1.603213</td><td>н</td><td>-4.178626</td><td>-0.716458</td><td>0.755326</td><td></td></t<>	н	4.964987	-2.744391	-1.603213	н	-4.178626	-0.716458	0.755326	
H 4.142179 2.168073 -1.829338 C -3.766110 -2.948843 -0.821793 H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C	н	2.500451	0.585438	-2.833854	н	-1.215325	-3.772718	-0.153266	4
H 6.586410 -1.168379 -0.571961 H -3.214978 -3.075266 -1.772095 C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -	н	4.142179	2.168073	-1.829338	С	-3.766110	-2.948843	-0.821793	
C 2.523489 2.308256 0.664808 H -4.639628 -2.298542 -0.997493 C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.6	н	6.586410	-1.168379	-0.571961	н	-3.214978	-3.075266	-1.772095	
C 1.370887 2.657984 -0.035611 H -4.124317 -3.942424 -0.486804 H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340 <td>с</td> <td>2.523489</td> <td>2.308256</td> <td>0.664808</td> <td>н</td> <td>-4.639628</td> <td>-2.298542</td> <td>-0.997493</td> <td></td>	с	2.523489	2.308256	0.664808	н	-4.639628	-2.298542	-0.997493	
H 1.116436 3.707618 -0.215602 C -0.010202 -0.531207 3.065899 C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.054320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	1.370887	2.657984	-0.035611	н	-4.124317	-3.942424	-0.486804	
C 0.447075 1.669368 -0.404826 H 0.993007 -0.775094 2.670099 C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.054320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	н	1.116436	3.707618	-0.215602	с	-0.010202	-0.531207	3.065899	
C 3.342494 3.433100 1.249074 C -0.157834 -1.231217 4.437158 H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.054320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	С	0.447075	1.669368	-0.404826	н	0.993007	-0.775094	2.670099	
H 4.314404 3.540169 0.735017 H 0.612229 -0.857014 5.137311 H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	3.342494	3.433100	1.249074	с	-0.157834	-1.231217	4.437158	
H 3.550615 3.256538 2.319312 H -0.041282 -2.327442 4.345822 H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	н	4.314404	3.540169	0.735017	н	0.612229	-0.857014	5.137311	
H 2.803748 4.391325 1.152081 H -1.154320 -1.024900 4.872791 C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	н	3.550615	3.256538	2.319312	н	-0.041282	-2.327442	4.345822	
C -0.881059 1.990717 -0.912390 C -0.115421 0.995128 3.200445 D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	н	2.803748	4.391325	1.152081	н	-1.154320	-1.024900	4.872791	
D -1.175897 3.146402 -1.503496 H 0.712614 1.371997 3.827711 C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	с	-0.881059	1.990717	-0.912390	с	-0.115421	0.995128	3.200445	
C -2.607907 3.077724 -1.827324 H -1.062366 1.292811 3.690340	о	-1.175897	3.146402	-1.503496	н	0.712614	1.371997	3.827711	
	с	-2.607907	3.077724	-1.827324	н	-1.062366	1.292811	3.690340	
Н -3.133778 3.787207 -1.163173 Н -0.058823 1.490828 2.215585	н	-3.133778	3.787207	-1.163173	н	-0.058823	1.490828	2.215585	

Table S11. Structure and Cartesian coordinates of (R_p, S, R_M) -7a.

С	-4.186411	-0.783590	1.298569	н	2.750264	-2.793737	-3.389095	
С	-2.345999	1.320735	0.591984	С	2.923690	-1.279125	-1.739513	
С	-2.959862	-1.126231	0.616424	н	3.068058	-0.542462	-2.554558	
С	-4.279629	0.501884	1.836112	С	4.170876	-1.319702	-0.886623	
С	-3.400618	1.546507	1.464646	С	6.477920	-1.317386	0.729067	
С	-2.002535	-0.053028	0.338262	С	5.362879	-0.733212	-1.352772	
н	-5.178922	0.766128	2.405567	С	4.142297	-1.927112	0.384892	
н	-3.678831	2.577250	1.719994	С	5.291551	-1.918896	1.190188	
С	-1.841975	2.423009	-0.322759	С	6.515343	-0.730568	-0.547749	
н	-0.940264	2.063741	-0.837250	н	5.386827	-0.267383	-2.347133	
н	-1.568514	3.324207	0.255287	н	3.208680	-2.357093	0.765800	
С	-5.495390	-1.567437	1.212796	н	5.259314	-2.380648	2.185042	
н	-6.202205	-1.088054	1.912739	н	7.439706	-0.269051	-0.916331	
н	-5.411758	-2.615647	1.539005	н	7.373865	-1.310886	1.362172	
С	-6.161397	-1.536387	-0.237911	Ν	-0.790821	-0.317574	-0.237839	
н	-7.258146	-1.524502	-0.095859	Ν	1.698258	-0.893846	-1.002697	
н	-5.913272	-2.466805	-0.781443	Ru	1.221792	0.395418	0.582609	
С	-2.905206	2.881904	-1.430938	CI	0.899349	-1.644782	1.906654	N I
н	-2.343558	3.049799	-2.369626	С	2.548372	2.070272	-0.094960	
н	-3.335238	3.853530	-1.127297	С	1.402891	1.555145	2.536918	
С	-4.015692	1.875059	-1.620600	С	3.247559	1.262383	0.874317	
С	-5.677867	-0.342936	-1.031551	С	1.301342	2.633519	0.291515	
С	-5.258508	2.057755	-0.980360	С	0.735672	2.365530	1.585471	
С	-3.742201	0.611365	-2.179708	С	2.674930	0.989717	2.141511	$(\Lambda \Lambda)$
С	-4.566445	-0.483433	-1.887637	н	4.183347	0.773548	0.592968	
С	-6.086509	0.962627	-0.693806	н	0.739712	3.232144	-0.427352	
н	-5.523088	3.052123	-0.596489	н	-0.264821	2.733859	1.825754	
н	-2.810439	0.453945	-2.739721	н	3.162645	0.265855	2.801407	
н	-4.267974	-1.486672	-2.218298	С	0.797416	1.218491	3.867369	
н	-6.987102	1.108967	-0.082521	н	0.888430	0.133164	4.054568	
С	-2.645253	-2.437555	0.111073	н	-0.270057	1.498115	3.899653	
С	-1.518285	-2.580351	-0.697182	н	1.330832	1.761935	4.672679	
н	-1.261507	-3.548744	-1.138422	С	3.133529	2.290979	-1.474907	
С	-0.598420	-1.524636	-0.802889	н	3.861704	1.475050	-1.636504	
С	-3.425934	-3.686236	0.440214	С	3.907725	3.627427	-1.498845	
н	-4.414983	-3.699078	-0.051787	н	4.388485	3.771427	-2.484489	
н	-3.594509	-3.762941	1.529100	н	4.693439	3.650273	-0.720750	
н	-2.873947	-4.582844	0.109875	н	3.220644	4.477383	-1.321791	
С	0.743211	-1.708825	-1.346231	С	2.072394	2.222260	-2.586798	
ο	1.046309	-2.697797	-2.182627	н	2.559455	2.245131	-3.578973	
С	2.505283	-2.664945	-2.322863	н	1.383092	3.087164	-2.541543	
н	2.915105	-3.501909	-1.728495	н	1.470753	1.299057	-2.497407	

Table S12. Structure and Cartesian coordinates of (R_p, S, S_M) -7a.

С	-3.869515	-0.566480	1.442194	н	3.426963	-3.646775	-1.889807	
С	-1.972442	1.418143	0.526299	с	3.443271	-1.617967	-0.939641	
С	-2.596982	-1.000628	0.910653	N	-0.365688	-0.352189	0.054315	
С	-3.985733	0.780923	1.776608	Ν	2.158327	-1.051316	-0.500498	
С	-3.070130	1.749625	1.312422	Ru	1.543531	0.806689	0.168437	
С	-1.610673	0.018912	0.494801	CI	1.345918	1.396042	-2.171794	
н	-4.913630	1.130820	2.245449	c	2.507896	0.530529	2.157937	
н	-3.341110	2.808388	1.415158	c	1.889616	3.017271	0.752978	
С	-1.473638	2.462077	-0.453468	c	1.261258	1.197581	2.333353	
н	-0.394379	2.406809	-0.624647	c	3.442420	1.125922	1.229297	
н	-1.696955	3.454856	-0.022228	c	3,135451	2.315001	0.519274	
С	-5.178080	-1.355106	1.385427	ĉ	0 973408	2 440269	1 664225	
Н	-5.930437	-0.755555	1.927291	н	0 481362	0 738998	2 947642	
Н	-5.145891	-2.327573	1.899956	н	4 371605	0 592648	0 999216	
С	-5.721977	-1.582578	-0.098858	н	3 820987	2 680823	-0 251286	
Н	-6.824472	-1.504867	-0.057362	н	-0 010399	2 897133	1 797955	
Н	-5.481381	-2.610361	-0.428317	Ċ	1 575358	4 253273	-0.036869	
С	-2.153434	2.375651	-1.903076	ц	0 575503	4.233273	0.207661	()
Н	-1.364327	2.063275	-2.608036	н	1 615671	4.047505	-1 117060	M A
Н	-2.476291	3.396592	-2.177712	н	2 330670	5.035637	0 171/22	
С	-3.308805	1.407409	-1.947712	Ċ	2.330070	-0 776069	2 8/386/	
С	-5.117851	-0.587757	-1.065040	ц	3 515602	-1 327261	2.043004	
С	-4.581105	1.761873	-1.451265	Ċ	1 620///0	-1.527201	3 121833	
С	-3.062825	0.047884	-2.222342	ц	1 038870	-2 642426	3 502557	
С	-3.961029	-0.937367	-1.789220	н	1 02083/	-1 8020/17	2 206189	
С	-5.476467	0.775798	-1.013972	н	0 968808	-1 199647	3 891651	
Н	-4.823712	2.821917	-1.296785	Ċ	3 648022	-0 486071	4 135293	
Н	-2.101280	-0.241844	-2.666383	н	3.961927	-1.433589	4.611524	1
Н	-3.696882	-1.997505	-1.899905	н	3.021477	0.073549	4.856099	1
н	-6.408295	1.072030	-0.513330	н	4.552632	0.115282	3,926075	
С	-2.252350	-2.383530	0.727568	н	4.206230	-1.401661	-0.168669	
С	-1.044080	-2.682285	0.103538	c	3,918252	-1.024650	-2.288156	
Н	-0.746559	-3.719521	-0.080693	н	3 872112	0.073642	-2 160799	
С	-0.125879	-1.661048	-0.183667	Ċ	5 372833	-1 447568	-2 551219	
С	-3.080520	-3.548385	1.214491	н	5.457339	-2.548220	-2.653730	
н	-4.010643	-3.663325	0.629918	н	6.046647	-1.128120	-1.732032	
н	-3.367220	-3.414786	2.272546	н	5,739200	-0.999429	-3.492785	
н	-2.509699	-4.488555	1.124272	c	2.993163	-1.400389	-3.455566	
С	1.245784	-1.969514	-0.567599	н	1.946159	-1.125145	-3.241322	
0	1.641689	-3.195888	-0.905554	н	3.051064	-2.481816	-3.688502	
С	3.107951	-3.139903	-0.965488	н	3.299961	-0.850026	-4.363202	
н	3.490403	-3.684518	-0.083104		5.255501	5.050020		

Table S13. Structure and Cartesian coordinates of (R_p, R, R_M) -8.

С	-3.888730 -0.350175 -1.63	005 _F	2.686607 4.38	6656	1.035077	
С	-2.035036 -1.539233 0.21	917	3.088206 2.28	1065	0.375136	
С	-2.724139 0.402073 -1.22	698 S	-0.596798 0.3	0022	0.044795	
С	-3.901921 -1.715043 -1.33	939	1.871566 1.46	1689	0.252089	
С	-3.013236 -2.296846 -0.40	413 R	u 1558842 -05	3194	-0.066781	
С	-1.753411 -0.243987 -0.33	689 .	1 1 1 3 3 9 8 6 0 0 7	5422	-2 376330	
н	-4.748688 -2.317625 -1.68	996	3 182106 -1 85	1158	-2.370330	
н	-3.222930 -3.311392 -0.04	728	1 999167 2 13	7650	1 696627	
С	-1.535478 -1.902280 1.59	741	2 001074 2 66	020	0.745172	
н	-0.568392 -1.414228 1.76	026	2.001374 -2.00	221/	-0.743173	
н	-1.393296 -2.995319 1.66	504	2 01/010 1 20	1200	1 521606	
С	-5.226216 0.252377 -2.05	899 2	1 250260 2 7	4330 E671	0.502000	
н	-5.865570 -0.586453 -2.38	643		7742	1 620244	
н	-5.156128 0.931160 -2.92	349	1.300330 -3.13	E020	0 122769	
С	-5.990426 1.010610 -0.87	665		0200	0.133708	
н	-7.069478 0.798456 -0.99	744 [0 425746 2 21	0290 4177	2.383975	
н	-5.859338 2.102426 -0.99	770 2	1 22/727 2 20	1/60	2 060450	
С	-2.515505 -1.459335 2.79	538	0 422501 2 0	7022	3.003430	()
н	-1.916617 -0.870333 3.51	727 [7923	3.034270	
н	-2.854974 -2.373272 3.31	940 [1633	3.505102	
С	-3.704457 -0.663008 2.31	836 2	2.030310 -2.0	1031	3.071300	
С	-5.472630 0.580873 0.47	306	2 001656 1 90	2031	2.236301	
С	-4.881334 -1.317882 1.89	669	A 912194 2 01	1666	-3.000413	
С	-3.564611 0.703554 2.00	315	E 2020/0 2 03	1000	2 244084	
С	-4.442177 1.317708 1.09	526	1 255362 -3.03	10/18	-3.344984	1 71
С	-5.757735 -0.703097 0.98	441	5 609845 -2 97	2755	-1 580837	
н	-5.048932 -2.363440 2.18	935		1851	-2 /81686	Y
н	-2.689966 1.256444 2.36	469	5 051359 -0.4	7512	-3 5087/15	
н	-4.244626 2.345157 0.76	550	5 502018 -0 36	1778	-1 789167	
н	-6.598993 -1.274797 0.57	329	3 962507 0 39	1999	-2 375512	1
С	-2.487929 1.778788 -1.56	793 ·	3.771052 2.00	9728	-0.451647	
С	-1.406381 2.425580 -0.97	618	3.833794 2.08	6778	1,717730	
н	-1.196914 3.477862 -1.19	148	. 5.055754 2.00	1576	1 69//65	
С	-0.463931 1.688637 -0.23	125	5 032847 3 04	6625	1 809469	
С	-3.296134 2.561976 -2.57	372	. <u>4.704705</u> 4.10	1886	1.876677	
н	-4.310990 2.789588 -2.20	433 .	5.697075 2.94	8789	0.928941	
н	-3.405820 1.992997 -3.51	710	5.628534 2.82	9401	2.714849	
н	-2.799019 3.520050 -2.80	081 0	2.890935 2.20	4460	2.923584	
С	0.854074 2.244218 0.04	847	2.071901 1.46	3590	2.856178	
ο	1.083423 3.553194 0.01	063 .	2.436683 3.21	3020	2.982703	
С	2.525920 3.727654 0.16	273 .	3.444669 2.03	6452	3.865702	
н	2.903856 4.217426 -0.74	167 '		5452	3.003/02	

Table S14. Structure and Cartesian coordinates of (R_p, R, S_M) -8.

С	3.721143 0.5952	291 1.385048	H 2 971040 2 569775 2 220942
С	1.917716 -1.4251	LO7 0.371520	(-3.465432) = 1.502722 = 1.361859
С	2.472585 1.0044	155 0.782528	0
С	3.850416 -0.7519	911 1.721236	N 0.2709/27 0.90600 0.010175
С	2.987161 -1.7404	1.201560	N -2.200422 0.373013 -0.010301
С	1.528150 -0.0361	L92 0.335637	KU = 1.550500 = 0.002557 = 0.007/81
н	4.760960 -1.0813	343 2.236516	(1 - 1.3/1417 - 1.320833 - 2.430863)
н	3.279935 -2.793	099 1.305787	C = 1.489098 = 1.084569 = 2.154304
С	1.465275 -2.4616	644 -0.638152	C -2.3964485 -2.652401 0.183533
н	0.394167 -2.4005	505 -0.856602	C -0.926866 -2.2/3/23 1.55/961
н	1.672571 -3.4594	469 -0.209677	C -2.816355 -0.730478 1.777907
С	5.014684 1.4091	LO7 1.395680	C -3.543003 -1.511661 0.808810
н	5.744271 0.8351	1.993405	C -1.629032 -3.029891 0.594858
н	4.928826 2.3889	972 1.889295	H 0.111562 -2.528547 1.788309
С	5.645644 1.6249	38 -0.058535	H -3.263271 0.191184 2.160309
H	6.743209 1.5402	254 0.047029	H -4.536602 -1.188505 0.483793
н	5.431682 2.6531	68 -0.404188	H -1.133494 -3.864113 0.090062
c	2.201866 -2.3516	593 -2.058793	C -3.669853 -3.414318 -0.892899
н	1.438338 -2.037	544 -2.791186	H -2.990766 -3.550116 -1.754240
н	2 545561 -3 366	105 -2 332652	H -4.571541 -2.878850 -1.236434
Ċ	3 3/9/89 -1 372	65 -2 0/37/6	H -3.970041 -4.411717 -0.514700
ĉ	5 095783 0 6305	32 -1 057119	C -0.653798 -0.274470 3.124674
ĉ	1 500287 1 720	17 1 A9967A	H 0.402507 -0.439722 2.836343
ĉ	2 107102 0 0120	17 -1.488024 67 .7 271602	C -0.849483 -0.825221 4.555110
ĉ	3.10/102 -0.0123	07 1 020506	H -0.191704 -0.287507 5.263257
č	5.373438 0.3733 E 461737 0 7209	07 -1.030300	H -0.609798 -1.903833 4.608550
L L	4 942270 2 770	700 1 220/67	H -1.898083 -0.687975 4.882536
	4.0452/0 -2.//5	20 -1.550407	C -0.933012 1.234845 3.053037
	2.100918 0.2/20		H -0.205977 1.782376 3.679557
	6 260626 1 022		H -1.943971 1.477543 3.432002
	0.309020 -1.0230		H -0.850497 1.601615 2.014970
C	2.121935 2.3770	0.554774	H -3.889247 0.748835 -2.049500
с 	0.961985 2.6375		C -4.490755 1.829525 -0.246752
н	0.6/5343 3.6620	0.449580	H -4.685331 0.874662 0.274091
C	0.068089 1.5962	14 -0.481322	C -5.813199 2.308198 -0.867999
C	2.901340 3.56/6	33 1.038398	H -6.572208 2.472809 -0.081459
н	3.865420 3.6786	533 0.510649	H -6.213184 1.567936 -1.587124
н	3.122535 3.4684	46/ 2.115881	H -5.678953 3.268409 -1.403458
н	2.325364 4.4962	260 0.884004	C -3.938626 2.830838 0.779909
С	-1.271628 1.8524	173 -0.993786	H -2.996155 2.469397 1.230678
0	-1.595638 2.9712	236 -1.636170	H -4.671438 2.990380 1.592212
С	-2.956326 2.7496	568 -2.144974	H -3.741362 3.816191 0.315732
н	-3.537912 3.6658	352 -1.954523	

Table S15. Structure and Cartesian coordinates of (R_p, S, R_M) -9.

ооооонноннонноннонносооооннносноонннооон

-3.771799 -1.032702 1.435639	H 2 859491 -1 839497 -3 602755	
-1.999729 1.174229 0.925640	C 3.326679 -1.482803 -1.451080	
-2.573212 -1.260428 0.662248	N -0.462115 -0.294075 -0.208816	
-3.852966 0.164378 2.148067	N 2 066906 -0 917530 -0 937604	
-3.000797 1.259553 1.881547	Ru 1 695273 0 485367 0 527372	
-1.645596 -0.139369 0.461028	Cl 1 206853 -1 345009 2 036154	
-4.724329 0.333017 2.792742	C = 2.011053 = 2.030134	
-3.257108 2.239419 2.304393	C = 2.011033 = 2.033318 = 0.143123	
-1.535105 2.403420 0.187257	C 3.17/E70 1.991738 0.30060	
-0.537862 2.209555 -0.217532	C = 3.174370 = 1.881728 = 0.330800	
-1.473856 3.255222 0.888182	C = 1.490038 = 2.070134 = 1.198919	
-5.077237 -1.814658 1.296986	C = 2.080307 = 1.938231 = 2.242722	
-5.759272 -1.437808 2.079172	H = 2 = 71166 + 1 = 207526 + 1 = 409082	
-4.976161 -2.895007 1.480935		
-5.798755 -1.605124 -0.112965		
-6.887958 -1.577258 0.076692		
-5.604731 -2.478773 -0.762212		
-2.480616 2.841025 -1.037379		
-1.847802 2.902396 -1.941528	H 4.551500 -0.415475 2.080278	
-2.863004 3.856421 -0.828068	H 3.127533 -0.173511 3.085108	
-3.626998 1.883882 -1.256660	H 4.472043 1.023092 3.749184	
-5.313601 -0.347450 -0.800522		V I /
-4.827830 2.028390 -0.530926	C 0.006157 2 560425 2 469212	
-3.421112 0.678893 -1.956126		
-4.258277 -0.422674 -1.731355		"
-5.663733 0.925981 -0.305998	H 0.2/2/88 1./93311 -2.100240	
-5.045761 2.983941 -0.035552	П 1.865858 2.000055 -2.865204 С 2.246919 4 E09324 1 70E907	
-2.528541 0.562653 -2.585456		1
-4.010654 -1.390697 -2.185947	H 1.802284 5.250767 -2.472470	*.
-6.525118 1.027671 0.367510	H 3.276595 4.184399 -2.141072	
-2.263872 -2.500525 0.004130		
-1.151666 -2.537779 -0.832549	H 3.974057 -0.007822 -1.825091	
-0.883890 -3.454238 -1.368385		
-0.257767 -1.453065 -0.861857	H 4.125017 -1.589665 0.522343	
-3.025839 -3.788489 0.200379		
-4.026765 -3.749802 -0.265950	H 8.075328 -3.104208 -0.027407	
-3.166719 -3.999653 1.275321	H 0.00581/ -1.0530/1 -1.082288	
-2.476387 -4.632298 -0.251270	H 5.5048/6 -3.233/20 -1./12183	
1.081737 -1.624116 -1.405149		
1.380810 -2.546076 -2.319253	н 2.318013 -3.301980 0.444970	
2.802551 -2.353416 -2.625841	н з.8/6/// -3.994324 0.953978	
3.273119 -3.347068 -2.691179	н з.298983 -4.293/49 -0.705097	

Table S16. Structure and Cartesian coordinates of (R_p, S, S_M) -9.

С	-3.620160	-0.725457	1.462996	С	2.887294	-2.873671	-2.297583	
С	-1.739943	1.360028	0.762336	н	3.328096	-3.638395	-1.628910	
С	-2.417829	-1.073988	0.739599	н	3.056745	-3.148060	-3.351433	
С	-3.655766	0.535544	2.054862	С	3.358033	-1.426439	-1.947890	
С	-2.750957	1.558544	1.695965	Ν	-0.251914	-0.314276	-0.185986	
С	-1.437514	-0.013263	0.435966	Ν	2.208073	-0.972575	-1.104092	
н	-4.525111	0.807283	2.666169	Ru	1.711660	0.691691	0.087722	
н	-2.974180	2.583604	2.018789	CI	1.450027	1.833857	-2.028045	
С	-1.284934	2.552664	-0.056155	С	2.512001	-0.082201	2.033958	
н	-0.212687	2.536362	-0.282354	С	2.293325	2.680087	1.099915	
н	-1.491889	3.460300	0.540303	С	1.342956	0.698157	2.268143	
С	-4.956277	-1.464079	1.382124	С	3.567745	0.553242	1.289266	
н	-5.633352	-0.969288	2.100301	С	3.460334	1.883400	0.798444	
н	-4.909850	-2.518552	1.694301	С	1.255065	2.070335	1.848856	
С	-5.641974	-1.388380	-0.059497	н	0.467135	0.242317	2.738189	
н	-6.729601	-1.270473	0.102551	н	4.447931	-0.039103	1.029920	T
н	-5.495382	-2.347790	-0.589867	н	4.248147	2.296716	0.160816	
С	-2.027995	2.687413	-1.467884	н	0.333333	2.624400	2.037462	
н	-1.289944	2.428764	-2.246217	С	2.165582	4.071014	0.553379	
н	-2.300588	3.751556	-1.593641	н	1.209897	4.534028	0.850493	
С	-3.236566	1.790596	-1.576834	н	2.214933	4.033959	-0.551812	
С	-5.067429	-0.260025	-0.887444	н	3.000451	4.699254	0.919353	
С	-4.438557	2.099077	-0.904721	С	2.658355	-1.524234	2.475400	
С	-3.094976	0.495568	-2.112301	н	3.235442	-2.033283	1.677272	
С	-4.004075	-0.517078	-1.774378	С	1.313312	-2.251956	2.627968	
С	-5.343206	1.085019	-0.561648	н	1.484864	-3.325265	2.827011	4
н	-4.606398	3.121764	-0.541021	н	0.699557	-2.154033	1.715281	
н	-2.197410	0.254386	-2.697001	н	0.735030	-1.846115	3.479831	
н	-3.810479	-1.548826	-2.096024	С	3.486744	-1.584804	3.778358	
н	-6.208112	1.321345	0.072825	н	3.657435	-2.636529	4.074898	
С	-2.144656	-2.398371	0.252176	н	2.948241	-1.075830	4.600753	
С	-1.018723	-2.585759	-0.545422	н	4.470529	-1.093813	3.655845	
н	-0.785358	-3.568028	-0.968269	С	4.680607	-1.437056	-1.179049	
С	-0.090190	-1.546065	-0.709808	н	4.583946	-1.977275	-0.219413	
С	-2.965427	-3.621046	0.583660	н	5.454384	-1.939809	-1.788101	
н	-3.950398	-3.601412	0.083401	н	5.019972	-0.403760	-0.991962	
н	-3.146183	-3.693134	1.670747	С	3.469118	-0.556742	-3.211349	
н	-2.441236	-4.535293	0.256011	н	4.276796	-0.960625	-3.850980	
С	1.217716	-1.786119	-1.309178	н	3.698385	0.487359	-2.944516	
0	1.446764	-2.865441	-2.057717	н	2.519977	-0.560942	-3.775074	

Table S17. Structure and Cartesian coordinates of (R_p, R_M) -10.

С	-3.742040	-0.637091	1.457848	С	2.559598	-2.906642	-2.578133	
С	-1.753888	1.341573	0.818569	н	2.914544	-3.950191	-2.564250	
С	-2.570498	-1.034777	0.712793	н	2.641390	-2.490134	-3.600424	
С	-3.711356	0.612930	2.078887	С	3.244798	-1.998540	-1.510711	
С	-2.756668	1.598694	1.742466	Ν	-0.367599	-0.351356	-0.192059	
С	-1.531183	-0.031141	0.457699	Ν	2.065061	-1.230609	-1.015022	
н	-4.566563	0.912546	2.697022	Ru	1.801576	0.118059	0.569354	
н	-2.926136	2.629776	2.078349	Cl	1.212784	-1.846166	1.881597	
С	-1.169127	2.454250	-0.017931	С	2.383590	2.297903	0.072152	
н	-0.197626	2.128016	-0.400581	С	3.263396	0.563385	2.237278	
н	-1.021650	3.353637	0.606632	С	3.482729	1.412288	-0.093065	
С	-5.115679	-1.300399	1.365180	С	1.701447	2.262583	1.340231	
н	-5.758767	-0.807379	2.115083	С	2.116573	1.419884	2.398708	
н	-5.115741	-2.369902	1.625628	С	3.928473	0.566860	0.975729	
С	-5.816870	-1.123924	-0.061147	н	3.981209	1.361640	-1.063519	
н	-6.896404	-0.967992	0.121057	н	0.812133	2.878509	1.481918	IT I I I I I I I I I I I I I I I I I I
н	-5.717453	-2.059687	-0.641196	н	1.535011	1.374006	3.324199	(1
С	-2.066121	2.883919	-1.281331	н	4.760382	-0.124326	0.814453	M ·
н	-1.425784	2.815748	-2.180083	С	3.727035	-0.319510	3.356463	
н	-2.348633	3.944593	-1.153919	н	4.317694	-1.170933	2.978301	
С	-3.299840	2.029404	-1.440653	н	2.868085	-0.713003	3.924925	
С	-5.205243	0.020431	-0.839080	н	4.366005	0.278769	4.037774	
С	-4.486728	2.350617	-0.749297	С	1.992555	3.240530	-1.051757	
С	-3.209687	0.757673	-2.039100	н	1.080734	3.776909	-0.735441	
С	-4.155705	-0.233202	-1.744555	С	1.680812	2.477797	-2.354100	
С	-5.429720	1.357258	-0.450908	н	1.353910	3.182304	-3.140832	\sim
н	-4.613415	3.360199	-0.336115	н	0.889554	1.723671	-2.192845	
н	-2.326589	0.502871	-2.640141	н	2.579637	1.951085	-2.727482	•
н	-4.002842	-1.254130	-2.116938	С	3.105075	4.292150	-1.263360	
н	-6.282457	1.596916	0.198270	н	2.795286	5.017777	-2.038147	
С	-2.394574	-2.332146	0.116771	н	4.042782	3.809886	-1.600627	
С	-1.316807	-2.515005	-0.744572	н	3.318190	4.847078	-0.330785	
н	-1.159956	-3.472715	-1.250683	С	3.809602	-2.831265	-0.346567	
С	-0.308980	-1.537635	-0.823901	н	3.033886	-3.496600	0.070630	
С	-3.267533	-3.530393	0.397742	н	4.140849	-2.167210	0.467922	
н	-4.265064	-3.435106	-0.067922	н	4.667809	-3.432303	-0.701115	
н	-3.416583	-3.657824	1.484491	С	4.318427	-1.115579	-2.156034	
н	-2.798644	-4.447321	0.001107	н	5.028004	-1.753980	-2.714822	
С	0.993458	-1.867393	-1.388095	н	4.900518	-0.569291	-1.395481	
ο	1.147851	-2.900008	-2.216059	н	3.865028	-0.394806	-2.860414	

Table S18. Structure and Cartesian coordinates of (R_p, S_M) -10.

Analysis of the electronic transitions

In order to verify which kind of electronic transitions occur above the 250 nm and which role can be attributed to the Ru atom, we report hereafter a detailed analysis of some of them in terms of molecular orbital composition for (R_p ,R, R_M)-8. Compound 8 has been chosen as a representative of all complexes. Since length and velocity formalisms provide quite similar results, we focus only on the data computed for the velocity formalism.



Figure S7. Calculated (B3LYP/SV(P)) ECD spectra of (R_p, R, R_M) -8. Rotational strengths larger than 20×10^{-40} erg esu cm Gauss⁻¹ have been indicated using the enumeration of the calculation.

Apart the HOMO (170), which is localized almost exclusively on the paracyclophane unit, all others highest occupied MOs shown below are delocalized on Ru (d orbitals), Cl (p orbitals) and ligands (π orbitals). With the exception of MO 174, all other relevant occupied orbitals are delocalized on Ru, Cl, p-cymene and the two aromatic parts of quinolinophane. Some of the relevant virtual orbitals are slightly more localized. MO 171, 172 and 175 lack appreciable electron density of the phenyl part of the quinolinophane;

MO 176 lack density on all the quinolinophane and MO 174 lack density on chlorine and the metal. Therefore, Cotton effects above 250 nm are attributable to metal-to-metal (MM) d-d transitions, metal-toligand and ligand-to-metal charge transfer, and $\pi - \pi^*$ transitions.

Excited State	Wavelength (nm)	Rotational strength $(10^{-40} \text{ erg esu} \text{ cm Gauss}^{-1})$	Largest contributions
2	515	21.3	$169 \rightarrow 171$ $168 \rightarrow 171$
3	483	-44.0	$167 \rightarrow 171$ $167 \rightarrow 172$
5	451	64.9	$168 \rightarrow 171$ $169 \rightarrow 171$
7	422	-24.0	$167 \rightarrow 171$ $167 \rightarrow 172$
14	351	-21.3	164→171 168→172
20	326	20.9	168→174
27	302	48.4	$166 \rightarrow 174$ $164 \rightarrow 172$ $162 \rightarrow 171$
34	275	-23.2	$170 \rightarrow 176$ $167 \rightarrow 176$ $162 \rightarrow 171$
35	274	21.7	$170 \rightarrow 177$ $162 \rightarrow 171$ $170 \rightarrow 176$
44	258	-31.9	$164 \rightarrow 174$ $166 \rightarrow 175$
49	250	-32.4	$162 \rightarrow 172$ $163 \rightarrow 172$

Table S19. Analysis of the most important rotational strengths calculated at B3LYP/SV(P) level above the 250 nm.



Figure S8. Isosurfaces (0.02 a.u.) of some selected MOs.



Figure S9. Isosurfaces (0.02 a.u.) of some selected MOs.

Pearson's correlation coefficient (PCC)

Pearson's correlation coefficient r has been computed according to the formula

$$r = \frac{n \sum x_{i} y_{i} - \sum x_{i} \sum y_{i}}{\sqrt{n \sum x_{i}^{2} - (\sum x_{i})^{2}} \sqrt{n \sum y_{i}^{2} - (\sum y_{i})^{2}}}$$

where x_i , y_i (for i=1,2,...n) are data set points, that is, circular dichroism values, taken from experimental and theoretically predicted spectra of a given complex respectively. In order to find the best resemblance between experimental and theoretical spectra, it is customary to apply a wavelength shift w_s to the predicted data; hence, PCC can be thought as a function of the shift, i.e., $r=r(w_s)$.

In the following a series of plots is reported where r is analyzed with respect to a varying blue-shift from -50 nm to 50 nm. For each complex four PCC's were determined, that is, for the length and velocity formalism and for both Ru configurations. PCC's are computed summing over the whole range of experimental wavelengths (200 nm - 600 nm) in step of 0.1 nm as collected by the instrument.

It can be observed that: i) length and velocity formalism do not deviate appreciable; ii) the *R* configuration at Ru provides the largest positive correlation in all cases for a moderate negative blue-shift, i.e., a red-shift; iii) for all complexes, the *S* configuration at Ru provides a negative correlation where the PCC for the R configuration is maximum.



Figure S10. PCC's of 7a as a function of blue-shift.



Figure S11. PCC's difference between R_M and S_M configuration of **7a** as a function of blue-shift.



Figure S12. PCC's of 6a as a function of blue-shift.



Figure S13. PCC's difference between R_M and S_M configuration of **6a** as a function of blue-shift.



Figure S14. PCC's of 8 as a function of blue-shift.



Figure S15. PCC's difference between R_M and S_M configuration of **8** as a function of blue-shift.



Figure S16. PCC's of 9 as a function of blue-shift.



Figure S17. PCC's difference between R_M and S_M configuration of **9** as a function of blue-shift.



Figure S18. PCC's of 10 as a function of blue-shift.



Figure S19. PCC's difference between R_M and S_M configuration of **10** as a function of blue-shift.

X Ray crystallography section

A single crystal of (R_p, S) -[QUINOPHOX]⁺ PF₆⁻ suitable for X-ray diffraction (a red block) with approximate dimensions of 0.18 mm × 0.14 mm × 0.12 mm), was obtained by crystallization from dichloromethane.

Data were collected on a XCALIBUR (Kuma4CCD) diffractometer using Mo-K α graphite monochromated radiation ($\lambda = 0.71069$ Å), ω scans and the frame data were acquired with the CRYSALIS (CCD 171) software.¹ The crystal to detector distance was 65.77 mm.

The structure was solved using direct methods and refined against $|F|^2$.

The Laue symmetry was determined to be 2/m. The dimensions of the cell yield a calculated density to 1.538 g cm⁻³ (Z = 2 and FW = 919.15) and the investigation of the observed systematic absences are consistent with the monoclinic space group *P21* (no. 4). The data were collected at room temperature. The lattice parameters are: a = 12.3597(9), b = 11.3107(8) and c = 14.8410(10) Å, $\beta = 106.960(5)$, and V = 1984.5(2) Å³. Data were collected to $2\theta_{max}$ of 56.70° in the index ranges $-17 \le h \le 17$, $-13 \le k \le 15$, and $-21 \le l \le 20$ with a total of 18065 reflections collected of which 0 rejected and 9895 are unique reflections independent *R*(int) = 0.0279, up to a resolution of 0.69 Å.

The frames were then processed using the CRYSALIS (RED 171) software to give the *hkl* file corrected for scan speed, background, and Lorentz and polarization effects. Standard reflections, measured periodically, showed no apparent variation in intensity during data collection, therefore, no correction for crystal decomposition was necessary. The data were corrected for absorption using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.¹

The structure was solved by the direct method using the Sir97² program and refined by the full-matrix leastsquares method on F^2 using SHELXL-97³ WinGX⁴ version. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were added at the calculated positions and refined using a riding model.

The final cycle of full-matrix least-squares refinement against $|F|^2$ was based on 7906 observed reflections $[F_0 > 4 \sigma (F_0)]$ and 483 variable parameters and converged with unweighted and weighted agreement factors of R = 0.0468 and $R_w = 0.0719$, and GOF = 0.923.

 $(w=1/[\s^2^{(Fo^2^)}+(0.0675P)^2+0.0000P]$ where $P=(Fo^2^+2Fc^2)/3')$.

The absolute configuration was determined by the Flack parameter determinate with SHELXL-97. The value obtained was quite definitive, but as a further check it has been also determined correctly, using the TWIN and BASF commands of the program.

Finally the PF_6^- anion is positioned on the opposite side of the paracyclophane moiety. It shows a disorder probably ascribable to its thermal movement, so it is impossible to determine exactly the position of the fluorine atoms. A better determination could be obtained at low temperature, but that it was not possible to perform not having available the necessary instrumentation.

For better resolution, based on experimental evidence, we have hypothesized two conformations of the PF6 with the same probability of existence (0.5). The distance P-Ru is of 5,729 Å. In the crystal unit cell a molecule of dicloromethane (solvent) is present.



Figure S20. Thermal ellipsoid plot of (S_p, R, S_{Ru}) -7b complex with significant bond length and angles

References

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