Mechanistic identification and improvement of a direct enantioconvergent transformation in coppercatalyzed asymmetric allylic alkylation

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Supporting Information

- 1. General comments
- 2. Additional data
- 3. Experimental part
- 4. Spectroscopic and Chromatographic data

1. General comments

Nuclear magnetic resonance spectra:

¹H, ¹³C and ¹⁹F NMR spectra were recorded either on ARX-300, AMX-400 or AM-500 Bruker Avance spectrometers. ²H NMR spectra were recorded on ARX-300 Bruker Avance spectrometers. ¹H, ²H and ¹³C NMR chemical shifts (δ) are given in ppm relative to SiMe₄. ¹⁹F NMR chemical shifts (δ) are given in ppm relative to CFCl₃. Peaks multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), dt (doublet of triplet), ddd (doublet of doublet of doublet), td (triplet of doublet), qd (quartet of doublet), brs (broad signal). Coupling constants are reported in Hertz (Hz).

Optical activity:

Optical rotations were recorded on a Perkin-Elmer 241 polarimeter at 25 °C in a 10 cm cell in the stated solvent; $[\alpha]_D$ values are given in 10^{-1} deg.cm² g⁻¹ (concentration c given as g/100 mL).

Enantiomeric excesses:

Enantiomeric excesses were determined by GC on chiral stationary phase. The measurements were recorder either on a HP6890 (H₂ as vector gas) or HP6850 (H₂ as vector gas) with stated stationary phase. Temperature programs are described as follows: initial temperature (°C) - initial time (min) - temperature gradient (°C/min) - final temperature (°C); retention times (R_T) are given in minute.

Chromatography:

Analytical thin layer chromatography (TLC) was performed on Merck silica gel 60 F_{254} supported on aluminium sheets. TLC traces were visualized by UV lamp (254 nm) or with potassium permanganate (KMnO₄) stain. Flash chromatography was performed using silicagel 32-63 µm, 60 Å from Fluka.

IR spectra:

IR spectra measurements were recorded on a Perkin-Elmer 1650 FT-IR spectrometer using neat samples. Wavenumbers are given in cm⁻¹.

Mass spectrometry:

Mass spectrometry analyses were mainly achieved by electronic impact (EI) on a double-focusing magnetic sector mass spectrometer (geometry BE), MAT 95 from Finnigan. The measurements were performed at the University of Zürich. Few analyses were obtained by electrospray ionization (ESI) and were performed on QqTOF, QStar pulsar or XL instrument from AB/MDS Sciex. The measurements have been done at the University of Geneva by the Science Mass Spectrometry team.

Reagent and solvent:

All reactions were carried out with flame-dried glassware. Solvents were dried by filtration over alumina previously activated at 350 °C during 12 hours under nitrogen before use. CuTC was purchased from FrontierScientific and used as received. All chiral ligands were prepared according to litterature procedures.¹ Chiral amines used for the preparation of phospharamidite ligands were given by BASF.

¹ For phosphoramidite ligands L1 and L2, see: A. Alexakis, D. Polet, S. Rosset, S. March, *J. Org. Chem.* 2004, *69*, 5660.

Computational investigations:

All calculations have been performed with Gaussian 03 package.² The density functional theory (DFT) method was employed using B3LYP hybrid functional.³ The structures were optimized in gas phase using 6-31G(d) for C H N O P Br atoms and LanL2DZ basis sets for Cu.⁴ All stationary points were characterized by vibrational analysis, and were confirmed to be part of the intrinsic reaction coordinate (IRC) of the reported pathways. Single point energy calculations have been performed in dichloromethane using the CPCM solvation model.⁵ Relative energies are corrected for enthalpy and entropy factors at -78 °C and are showed in units of kcal/mol. Distances and bond lengths are given in units of angströms (Å). All depicted structures were generated using CYLview program.⁶

2. Additional data

2.1. Computational investigations

2.1.1. Alkylation of (*R*)-1



For anti-S_N2' pathway

For anti-S_N2 pathway

Figure S1. Energy profiles corresponding to the alkylation of (*R*)-1 by MeCuL1 in both *anti*- S_N2' and *anti*- S_N2 pathways.

² M. J. Frisch *et al. Gaussian 03*, revision C. 02; Gaussian, Inc.:Wallingford, CT, 2004.

³ For B3LYP hybrid functional, see: a) C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785; b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623.

⁴ For 6-31G(d), see: a) W. J. Hehre, L. Radom, P. v R. Schleyer, J. A. Pople, *Ab Initio Molecular Orbital Theory*, John Wiley & Sons Inc. New York. 1986. For LanL2DZ, see: b) W. R. Wadt, P. J. Hay, *J. Chem. Phys.* **1985**, *82*, 284; c) P. J. Hay, W. R: Wadt, *J. Chem. Phys.* **1985**, *82*, 299.

⁵ For CPCM, see: a) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.* **2003**, *24*, 669; b) V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995.

⁶ C. Y. Legault, CYL*view*, 1.0b; Université de Sherbrooke, 2009; <u>http://www.cylview.org</u>.

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	ΔG (kcal/mol)
C1 _{(<i>R</i>)-SN2p}	-4977.210045	-4976.467738	-4976.445817	-4976.511307	0.0
$TS1_{(R)-SN2p}$	-4977.173301	-4976.431211	-4976.409806	-4976.472993	24.0
Int _{(R)-SN2p}	-2405.586869	-2404.844357	-2404.823780	-2404.885295	0.0
TS2 _{(R)-SN2p}	-2405.585323	-2404.842676	-2404.822418	-2404.883471	1.1
C2 _{(<i>R</i>)-SN2p}	-2405.655953	-2404.909699	-2404.889378	-2404.950933	-41.2

Table S1. Energy values of all stationary points relative to the anti-S_N2' pathway in gas phase

Table S2. Energy values of all stationary points relative to the *anti*-S_N2 pathway in gas phase

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
C1 _{(<i>R</i>)-SN2}	-4977.209006	-4976.467053	-4976.444879	-4976.511674	-0.2
TS1 _{(R)-SN2}	-4977.168410	-4976.426509	-4976.405008	-4976.469101	26.5
Int _{(R)-SN2}	-2405.582867	-2404.840654	-2404.819892	-2404.882433	1.8
$TS2_{(R)-SN2}$	-2405.581948	-2404.839415	-2404.819081	-2404.880391	3.1
$C2_{(R)-SN2}$	-2405.652006	-2404.906042	-2404.885538	-2404.948398	-39.6

Table S3. Energy values of all stationary points relative to the *anti*-S_N2' pathway in dichloromethane (CPCM)

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
C1 _{(<i>R</i>)-SN2p}	-4978.050351	-4977.308044	-4977.286123	-4977.351613	0.0
$TS1_{(R)-SN2p}$	-4978.036615	-4977.294525	-4977.273120	-4977.336307	9.6
Int _{(R)-SN2p}	-2406.468103	-2405.725591	-2405.705014	-2405.766529	0.0
$TS2_{(R)-SN2p}$	-2406.465726	-2405.723079	-2405.702821	-2405.763874	1.7
$C2_{(R)-SN2p}$	-2406.536391	-2405.790137	-2405.769816	-2405.831371	-40.7

Table S4. Energy values of all stationary points relative to the *anti*-S_N2 pathway in dichloromethane (CPCM)

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
$C1_{(R)-SN2}$	-4978.050097	-4977.308144	-4977.285970	-4977.352765	-0.7
$TS1_{(R)-SN2}$	-4978.032900	-4977.290999	-4977.269498	-4977.333591	11.3
$Int_{(R)-SN2}$	-2406.466158	-2405.723945	-2405.703183	-2405.765724	0.5
$TS2_{(R)-SN2}$	-2406.463340	-2405.720807	-2405.700473	-2405.761783	3.0
$C2_{(R)-SN2}$	-2406.533610	-2405.787646	-2405.767142	-2405.830002	-39.8

Cartesian coordinates of all stationary points:

	С	1.320422	2.664379	-3.469118	Н	-3.114091	-5.287855	-1.117084
- <u>\</u>	С	1 990831	3 579040	-2.613839	Н	-3 770469	-3 333647	0 224704
🤎 T 🖢	Ĉ	2.067401	2 207020	1 200060	11	0.222021	0 791667	2 429460
	C	2.00/401	5.297920	-1.208800	п	-0.225021	0./8100/	5.428400
	С	2.679947	4.272788	-0.372214	Н	0.147075	0.864911	-3.582592
	C	3 213023	5 431180	-0 894933	C	-2 167133	2 851833	-1 291613
	č	2 170002	5 (92046	0.091999		1 500952	2.031033	0.474105
	C	5.170992	3.083040	-2.283842	п	-1.309833	5.149/98	-0.4/4185
A CARLON AND A CAR	С	2.566900	4.773352	-3.123078	Н	-1.556739	2.501086	-2.126428
	н	2 508448	4 960543	-4 192757	Н	-2 717158	3 738210	-1 624609
	11	2.000110	(50(512	2 (95040	11	2.717150	1.59(0(0	1.757450
	н	3.001999	0.390313	-2.085940	н	-3./98830	1.580009	-1./5/459
° 5 b-1	Н	3.665429	6.161181	-0.229165	С	-4.221267	-0.930950	0.907117
	н	2 713352	4 104015	0.697716	н	-3 470368	-1 380764	1 564111
	11	1.200122	2.064707	4.527110	11	1.5(50(0	0.000/01	1.201111
C1 _{(R)-SN2p}	н	1.290123	2.804/8/	-4.55/118	н	-4.303009	-0.002080	1.3003/2
	Ν	-2.624718	0.463667	-0.480018	Н	-5.079114	-1.609140	0.836141
D 1 009759 0 010047 0 072565	C	-3 193192	1 796452	-0.865671	Н	-4 474056	-0 220269	-1.082865
P -1.098/58 0.01904/ 0.0/5565	č	4.14((2)	2.2(700)	0.102012	0	0.002401	1.000(20	1.2((200)
O -0.693516 1.384238 0.957622	C	-4.140021	2.30/980	0.183813	Cu	-0.802481	-1.990630	1.300290
C 0 584460 1 349685 1 513763	С	-3.713023	2.687508	1.479367	С	-1.449397	-2.080094	3.248810
C = 1.692401 = 1.661126 = 0.727492	C	-4 594607	3 249905	2 402006	н	-2 109399	-2 946959	3 404678
C 1.063401 1.001120 0.727462	č	5.000125	2 507502	2.102000	11	0.500120	2 107629	2 028027
C 2.991011 1.516271 1.320490	C	-5.922135	3.50/503	2.040501	н	-0.599129	-2.19/028	3.938027
C 3 100318 1 189909 2 714665	С	-6.361877	3.197273	0.760142	Н	-2.004009	-1.185887	3.566959
C = 4.397222 = 1.062074 = 2.204276	С	-5 477588	2 630672	-0 161732	С	0 166754	-3 989674	0 952508
C 4.387222 1.003074 3.304370	т П	5 0 20 10 1	2.020072	1 162022	Ĉ	0.454021	2 222021	0.151014
C 5.530133 1.211778 2.553263	п	-3.828484	2.391203	-1.103923	C	0.434031	-5.252021	-0.131814
C 5.427410 1.484205 1.169106	Н	-7.391853	3.390956	0.472044	Н	-0.237567	-3.197664	-0.988441
C 4 105236 1 633607 0 570673	Н	-6.606582	3.944621	2.768605	С	1.783488	-2.580320	-0.334120
-1.175250 + 1.055077 + 0.570075	н	-4 21/1354	3 488127	3 403022	Č	2 630001	-2 550222	0.93/107
н 4.139009 1.831601 -0.492919	11	-4.244334	3.40012/	1.76400022	č	2.050001	-2.339223	0.93419/
Н 6.328996 1.570743 0.568909	Н	-2.685608	2.484102	1.764209	C	1.178359	-4.332399	2.028258
H 6 508019 1 104794 3 014307	С	-3.652873	-0.639024	-0.488413	Н	0.875453	-3.865610	2.973430
II 0.300017 1.104/94 3.01439/	ć	-3 175635	-1 877150	-1 255811	ч	1 130215	-5 416410	2 202886
H 4.448946 0.828488 4.364396	č	-3.173033	-1.07/130	-1.233611		1.139213	-3.410410	2.202880
C 1.922099 0.961987 3.475072	C	-3.344452	-3.176963	-0.759872	C	2.610828	-3.916463	1.646590
C 0.685315 1.008446 2.881399	С	-2.971649	-4.289399	-1.522262	Н	-0.778676	-4.527863	0.979249
U 2.014020 0.715(07 4.520(00	C	-2 421912	-4 121805	-2 792357	н	1 693776	-1 598781	-0 792347
H 2.014020 0.715697 4.529689	c	-2.421712	-4.121005	-2.772557	11	1.075770	-1.576761	-0.792347
C 1.494695 2.078938 -0.690426	C	-2.248593	-2.8299/1	-3.299136	Н	3.651194	-2.245047	0.700333
C 0.744726 1.297351 -1.561647	С	-2.625001	-1.724211	-2.539575	Н	2.200830	-1.787544	1.592263
0 0.07((40 0.1(4))) = 1.140774	н	-2 482388	-0 724205	-2 940135	н	3 242272	-3 882577	2 541678
0 0.0/0040 0.10428/ -1.140//4	11	1 821105	2 6 9 5 6 2 4	4 207712	11	2.046611	1 665 410	0.074607
C 0.690295 1.561713 -2.952215	п	-1.821103	-2.083034	-4.28//12	п	5.040011	-4.003410	0.9/400/
	Н	-2.129021	-4.985525	-3.382602	Br	2.787127	-3.596557	-1.812281
	C	2 112277	0 670045	3 026450	ы	6 472067	1 020071	0 222225
•	C	-3.443277	0.670945	3.026459	Н	6.472067	-1.928871	-0.233325
• 54	C C	-3.443277 -3.534302	0.670945 0.905614	3.026459 1.613658	H H	6.472067 5.395157	-1.928871 0.090458	-0.233325 -1.117032
	C C C	-3.443277 -3.534302 -4.669854	0.670945 0.905614 1.610775	3.026459 1.613658 1.127400	Н Н Н	6.472067 5.395157 -0.940770	-1.928871 0.090458 1.670511	-0.233325 -1.117032 -3.482793
the the	C C C C	-3.443277 -3.534302 -4.669854 -5.666240	0.670945 0.905614 1.610775 2.034791	3.026459 1.613658 1.127400 1.980238	H H H H	6.472067 5.395157 -0.940770 -0.368153	-1.928871 0.090458 1.670511 -0.848743	-0.233325 -1.117032 -3.482793 3.110068
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Act	C C C C C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560	0.670945 0.905614 1.610775 2.034791 1.770406	3.026459 1.613658 1.127400 1.980238 3.367211	H H H C	6.472067 5.395157 -0.940770 -0.368153 0.164453	-1.928871 0.090458 1.670511 -0.848743 2.882978	-0.233325 -1.117032 -3.482793 3.110068 1.833198
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	C C C C C C H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 6.285211	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102602	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027007	H H H C H H	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 2.758200	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.400245
	C C C C C H H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997	H H H C H H H	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345
	C C C C C C H H H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326	Н Н Н С Н Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361
	C C C C C C H H H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146	Н Н Н С Н Н Н Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483
	C C C C C C H H H H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 0.299504	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384	Н Н Н С Н Н Н Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065
FS1/pr.sapr.	C C C C C C C C H H H H H	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384	Н Н Н С Н Н Н С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745020	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065
TS1 _{(P)-SN2p}	C C C C C C H H H H N	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410	3.026459 1.613658 1.127400 1.980238 3.367211 3.87410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377	Н Н Н С Н Н Н Н С Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833
TS1 _{(R)-SNZP}	C C C C C C C H H H H H N C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380	Н Н Н С Н Н Н Н Н Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724
F 0.695446 0.583010 -0.445041	C C C C C C C H H H H H H C C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120	Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н Н С Н Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н С Н Н Н С Н Н Н Н С Н Н Н С Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н Н С Н Н Н Н Н Н Н С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657
Р 0.695446 0.583010 -0.445041 О -0.489080 1.641758 -0.950396	C C C C C C H H H H N C C C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 0.682538	Н Н Н Н С Н Н Н Н С Н Н Н Н С Т	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.900202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 1.158150	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657
P 0.695446 0.583010 -0.445041 O -0.489080 1.641758 -0.950396 C 1 622174 1 066210 1 531408	C C C C C C H H H H H N C C C C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538	H H H C H H H H C H H H H H H C U	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188
P 0.695446 0.583010 -0.445041 O -0.489080 1.641758 -0.950396 C -1.622174 1.066319 -1.531408	C C C C C C C H H H H H N C C C C C C	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272	H H H C H H H H C H H H H C H H H C C H C H C H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H H C H H H H C H H H C H H H H C H H H C H H H H C H H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H H C H H H H C H	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217
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$FS1_{(R)-SN2p}$ P 0.695446 0.583010 -0.445041 O -0.489080 1.641758 -0.950396 C -1.622174 1.066319 -1.531408 C -2.590033 0.473162 -0.735167 C -3.685399 -0.187452 -1.408323 C -3.805246 -0.084746 -2.835701	C C C C C C C C H H H H H N C C C C C C	$\begin{array}{r} -3.443277\\ -3.534302\\ -4.669854\\ -5.666240\\ -5.589560\\ -4.497395\\ -4.416802\\ -6.385311\\ -6.516649\\ -4.741567\\ -2.266399\\ 1.774186\\ 1.537113\\ 1.848765\\ 1.133865\\ 1.407731\\ 2.396410\\ 3.110313\end{array}$	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526	Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н Н С И Н Н Н С И Н Н Н И С И И И И	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356
$F = 0.695446 \\ 0.583010 \\ -0.489080 \\ 1.641758 \\ -0.950396 \\ -0.489080 \\ 1.641758 \\ -0.950396 \\ -1.622174 \\ 1.066319 \\ -1.531408 \\ -2.590033 \\ 0.473162 \\ -0.735167 \\ -3.685399 \\ -0.187452 \\ -1.408323 \\ -3.805246 \\ -0.084746 \\ -2.835701 \\ -2.835$	СССССННННИ КСССССССС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938	Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н Н С С Н Н Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -3.889217 -4.348596 -4.386356 -3.984569
P 0.695446 0.583010 -0.445041 O -0.489080 1.641758 -0.950396 C -1.622174 1.066319 -1.531408 C -2.590033 0.473162 -0.735167 C -3.685399 -0.187452 -1.408323 C -3.805246 -0.084746 -2.835701 C -4.892538 -0.718992 -3.495303	ССССССН ННННNСССССС Н	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202	Н Н Н Н С Н Н Н Н С С Н Н Н С С Н Н Н С С Н Н Н С С Н Н Н С С Н Н Н С С И И И И	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -3.984569 -2.271334
$FS1_{(R)-SN2P}$ $P 0.695446 0.583010 -0.445041 \\ O -0.489080 1.641758 -0.950396 \\ C -1.622174 1.066319 -1.531408 \\ C -2.590033 0.473162 -0.735167 \\ C -3.685399 -0.187452 -1.408323 \\ C -3.805246 -0.084746 -2.835701 \\ C -4.892538 -0.718992 -3.495303 \\ C -5.812197 -1.462295 -2.792452 \\ \end{array}$	ССССССННННН КСССССССНН	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356 -3.984569 -2.271334 -0.891177
$F = 0.695446 = 0.583010 = 0.445041 \\ 0 = 0.489080 = 1.641758 = 0.950396 \\ C = 1.622174 = 1.066319 = 1.531408 \\ C = 2.590033 = 0.473162 = 0.735167 \\ C = 3.685399 = 0.187452 = 1.408323 \\ C = 3.805246 = 0.084746 = 2.835701 \\ C = 4.892538 = 0.718992 = 3.495303 \\ C = 5.812197 = -1.462295 = 2.792452 \\ C = 5.669657 = -1.609548 = -1.393220 \\ C = 5.669657 = -1.609548 = -1.39320 \\ C $	СССССННННИ КОСССССНН.	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067	Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н Н С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -3.984569 -2.271334 -0.891177
$F_{I,R} = 0.695446 + 0.583010 + 0.445041 + 0.09548 + 0.583010 + 0.445041 + 0.095396 + 0.187452 + 0.145042 + $	СССССННННИ ОСССССННН Н	$\begin{array}{r} -3.443277\\ -3.534302\\ -4.669854\\ -5.666240\\ -5.589560\\ -4.497395\\ -4.416802\\ -6.385311\\ -6.516649\\ -4.741567\\ -2.266399\\ 1.774186\\ 1.537113\\ 1.848765\\ 1.133865\\ 1.407731\\ 2.396410\\ 3.110313\\ 2.836867\\ 3.395836\\ 3.881524\\ 2.607053\end{array}$	$\begin{array}{c} 0.670945\\ 0.905614\\ 1.610775\\ 2.034791\\ 1.770406\\ 1.103728\\ 0.905861\\ 2.102692\\ 2.581894\\ 1.830553\\ -0.229504\\ 1.638410\\ 2.828499\\ 4.147113\\ 4.562810\\ 5.792856\\ 6.630022\\ 6.227685\\ 4.993271\\ 4.687149\\ 6.869472\\ 7.587764 \end{array}$	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.00062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -3.984569 -2.271334 -0.891177 -0.525255
$FS1_{(R)-SN2P}$ $P 0.695446 0.583010 -0.445041 \\ O -0.489080 1.641758 -0.950396 \\ C -1.622174 1.066319 -1.531408 \\ C -2.590033 0.473162 -0.735167 \\ C -3.685399 -0.187452 -1.408323 \\ C -3.805246 -0.084746 -2.835701 \\ C -4.892538 -0.718992 -3.495303 \\ C -5.812197 -1.462295 -2.792452 \\ C -5.669657 -1.609548 -1.393220 \\ C -4.639141 -0.989588 -0.720538 \\ \end{array}$	СССССННННН КССССССНННН	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137
$\begin{array}{c c} \hline & & & \\ \hline \hline & & \\ \hline$	СССССНННННИСССССССННННН	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.630553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169	Н Н Н Н С Н Н Н Н С И Н Н Н И С С Н Н Н С С Н С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 2.2.647483 -2.880442 -3.406406	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959
$\begin{array}{c} \\ \hline \\ $	СССССНННННКОСССССНННННС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226209	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 0.094412	Н Н Н Н С Н Н Н Н С С Н Н Н Н С С Н С С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.900202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959
$\begin{array}{c} \\ File \\ $	СССССНННННКСССССССНННННСС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С Н С С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712
$\begin{array}{c} \\ \hline \\ $	СССССННННН И СССССССННННН СС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С Н С С С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688
$\begin{array}{c} \\ \hline \\ $	СССССНННННИСССССССНННННССС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.10963 3.917376 1.473532 0.152036 -0.385602	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.098412 0.38865 -0.238149	Н Н Н Н С Н Н Н Н С С Н Н Н Н С С Н С С С Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.0151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.900062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193
$\begin{array}{c} \\ \hline \\ $	СОССОНННННКОСОССОНННННОСОС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С Н С С С Н Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.3408406 -3.970622 -3.3408406	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.27134 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054
$\begin{array}{c} \\ \hline \\ $	СССССНННННИСССССССНННННССССС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.396410 3.110313 2.396847 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.689953 5.675112	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С И С С С Н Н С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054
$\begin{array}{c} \hline & & & \\ \hline & &$	СССССНННННИССССССССНННННССССС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953 5.075112	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.630553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.098169 -0.098169 -0.098169 -0.098169 -0.098169 -0.238149 0.265243 1.394113	Н Н Н Н С Н Н Н Н С С Н Н Н Н С С Н С С С Н Н С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.0151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.900202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.840442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204
$\begin{array}{c} \\ \hline \\ $	СОССОНННННКОССССССННННКОСОСС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953 5.589533 5.5075112 3.940211	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950 -1.656669	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243 1.394113 2.023009	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н С С С С Н Н С Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.12520 1.059262 -0.146260 2.807394 1.127661	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100 -2.487652	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343
$\begin{array}{c} \\ \hline \\ $	СОСССНННННИССССССИНННННОССССС	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.396410 3.110313 2.396410 3.81524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.689953 5.075112 3.9402111 3.338669	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950 -1.656669	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.0790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243 1.394113 2.023009 1.526226	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С О С Н Н С Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394 1.127661 -0.809134	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100 -2.487652 -3.797382	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343 0.403250
$\begin{array}{c} \\ \hline \\ $	СОСССИННННИОСССССИНННННОССССИ	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953 5.075112 3.940211 3.338669 2.452266	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.630553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950 -1.656669 -0.498695 -0.498695 -0.498695	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243 1.394113 2.023009 1.526226	Н Н Н Н С Н Н Н Н С И Н Н Н И С С Н Н Н С С Н И С С И Н С И Н Н Н И	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394 1.127661 -0.809134 -0.915865	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.900202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.840442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100 -2.487652 -3.797382 -3.297582 -3.297582 -3.295755	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343 0.403250
$\begin{array}{c} \\ \hline \\ $	СОССОННННН КОСССССОНННННОСССССН:	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953 5.075112 3.940211 3.338669 2.452266	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 0.385602 -1.534647 -2.174950 -1.656669 -0.498695 -0.117796	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243 1.394113 2.023009 1.526226 2.022761	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н С С С С Н Н С Н Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394 1.127661 -0.809134 -0.915865	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.00062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100 -2.487652 -3.797382 -2.655755	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343 0.403250 -0.845184
$\begin{array}{c} \\ \hline \\ $	СССССНННННКСССССССНННННССССССННН	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.396410 3.110313 2.396847 0.365732 3.226298 3.835059 4.973293 5.589953 5.075112 3.940211 3.338669 2.452266 3.483480	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.830553 -0.229504 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950 -1.656669 -0.498695 -0.117796 -2.172640	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.28149 0.265243 1.394113 2.023009 1.526226 2.022761 2.862813	Н Н Н Н С Н Н Н Н С Н Н Н Н С С Н Н С С С С Н Н С Н Н Н Н Н Н Н Н Н Н Н С С Н С С С Н Н С Н Н Н Н Н Н	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394 1.127661 -0.809134 -0.915865 -1.128072	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.34834 -4.819075 -4.473180 -3.197100 -2.487652 -3.797382 -2.565755 -4.791294	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343 0.403250 -0.845184 -1.943411
$\begin{array}{c} \\ \hline \\ $	СОСССНННННКОСССССНННННОСССССНННН	-3.443277 -3.534302 -4.669854 -5.666240 -5.589560 -4.497395 -4.416802 -6.385311 -6.516649 -4.741567 -2.266399 1.774186 1.537113 1.848765 1.133865 1.407731 2.396410 3.110313 2.836867 3.395836 3.881524 2.607053 0.845847 0.365732 3.226298 3.835059 4.973293 5.589953 5.075112 3.940211 3.338669 2.452266 3.483480 5.544547	0.670945 0.905614 1.610775 2.034791 1.770406 1.103728 0.905861 2.102692 2.581894 1.638410 2.828499 4.147113 4.562810 5.792856 6.630022 6.227685 4.993271 4.687149 6.869472 7.587764 6.100963 3.917376 1.473532 0.152036 -0.385602 -1.534647 -2.174950 -1.656669 -0.498695 -0.117796 -2.172640 -3.077312	3.026459 1.613658 1.127400 1.980238 3.367211 3.874410 4.940541 4.027997 1.582326 0.068146 4.611384 0.269377 1.157380 0.450120 -0.683538 -1.281272 -0.755734 0.372526 0.967938 1.850202 0.790067 -1.223830 -2.159265 -1.098169 -0.094412 0.385865 -0.238149 0.265243 1.394113 2.023009 1.526226 2.022761 2.862813 1.775867	Н Н Н Н С Н Н Н Н С И Н Н Н И С С Н Н С С С С	6.472067 5.395157 -0.940770 -0.368153 0.164453 -0.650740 -0.016537 0.151242 2.273343 3.493167 3.139334 2.989724 4.563747 3.718730 1.451788 1.496789 2.439296 0.659602 1.383589 1.943114 2.136059 3.115220 1.032205 -0.299182 0.715577 0.123520 1.059262 -0.146260 2.807394 1.127661 -0.809134 -0.915865 -1.128072 0.332111	-1.928871 0.090458 1.670511 -0.848743 2.882978 2.990202 2.000062 3.758390 2.714024 1.810670 1.024219 2.745929 1.951322 2.263107 -1.158150 -0.702637 -1.016793 -1.204014 0.382089 -3.214601 -2.944295 -2.647483 -2.880442 -3.406406 -3.970622 -3.344834 -4.819075 -4.473180 -3.197100 -2.487652 -3.797382 -2.565755 -4.791294 -5.353861	-0.233325 -1.117032 -3.482793 3.110068 1.833198 1.116053 2.450096 2.490345 1.963361 -1.571483 -2.246065 -1.827833 -1.749724 0.483657 -1.953188 -3.889217 -4.348596 -4.386356 -3.984569 -2.271334 -0.891177 -0.525255 -0.040137 -0.482959 -2.750712 -3.430688 -3.358193 -1.577054 -2.929204 0.965343 0.403250 -0.845184 -1.943411 -1.131407

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		9	, î	С	-2.441534	1.803132	3.376348	Н	-0.487034	0.915793	3.536684
		1	9-Q	С	-3.549862	2.065945	2.528050	С	0.329812	3.398377	0.644746
	î	A a		С	-3 558565	1 536223	1 193742	н	-0 357778	3 248635	-0 188062
	1 38		$\sqrt{1}$	č	1 640062	1 991620	0.249524	и Ц	0.082706	2 022058	1 528245
			- Q -Q	C	-4.049002	1.001030	0.346324	11	-0.082790	2.923938	1.556245
	- W		200	C	-5.681314	2.672199	0.805327	Н	0.394653	4.473840	0.837265
-	178	Y 💓 💜	7 8	С	-5.687245	3.159696	2.132907	Н	2.354952	3.139796	1.219195
	Y There		6-9-0°	С	-4.638467	2.863436	2.972497	С	3.893786	0.582139	-1.122155
-	4 I -		1.	й	4 610173	3 247240	3 080787	й	3 495500	0 366070	1 /03270
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	a a		8 0	Н	-6.496814	2.928775	0.135256	Н	4.984527	0.499281	-1.082485
	1	nt		Н	-4.660082	1.529261	-0.676192	Н	3.864300	1.846787	0.574744
		(<i>R</i>)-SN2p		Н	-2.451796	2.188927	4.392153	Cu	1.112822	-1.988448	-0.916689
				N	1 894128	1 405108	0.185061	C.	1 964480	-2 354108	-2 686920
Р	0.754161	0.234611	-0.103995	C	1.004120	2.002157	0.105001		2.091205	-2.33+100	-2.000020
0	-0.320231	1 016710	-1.092817	C	1./45643	2.902157	0.338309	н	2.981305	-2.6/2492	-2.443277
č	-1 420040	0.229/36	-1.466550	С	2.351262	3.648605	-0.846605	Н	1.475939	-3.063644	-3.351431
č	-1.420040	0.227430	-1.400330	С	1.812762	3.533647	-2.137493	Н	1.946010	-1.345646	-3.108896
C	-2.462480	0.032492	-0.5/4145	С	2.359621	4.254750	-3.198362	С	0.541729	-3.966592	-1.051462
С	-3.510260	-0.878946	-0.968332	Č	3 1/10036	5 104455	-2.986/33	Č	-0.2388/19	-3 470166	0.068/02
С	-3.501473	-1.435834	-2.293378	c	2.000022	5.104455	1 70(507	c	0.23004/	-3.470100	1.251.450
С	-4 541887	-2.320518	-2.687715	C	3.989032	5.228902	-1./0059/	C	0.228464	-3.362343	1.351459
č	5 5378/1	2.627736	1 808505	С	3.441703	4.502950	-0.645009	С	1.674485	-4.917801	-0.749486
č	-5.557041	-2.077750	-1.000375	Н	3.863928	4.611356	0.352181	Н	1.227878	-5.918290	-0.625465
C	-5.526002	-2.16/049	-0.489297	Н	4.834064	5.888433	-1.530563	Н	2.354353	-4.991702	-1.603786
С	-4.543196	-1.291863	-0.080393	н	3 872502	5 666356	-3 81/300	C	2 433075	-4 515475	0 523789
Η	-4.552200	-0.913204	0.934602	11	1.021502	4 150050	4 1025(9	č	2.435075	4.313473	1 7101(7
Н	-6.300723	-2.467912	0.210050	н	1.951592	4.139039	-4.192308	U T	1.494813	-4.270000	1./1910/
н	-6 326406	-3 356305	-2 119711	Н	0.963276	2.879050	-2.310325	Н	1.196134	-5.224283	2.186446
11	-0.520400	-3.330373	-2.11)/11	С	3.328363	0.946091	0.256698	Н	3.172023	-5.280728	0.781019
Н	-4.529/61	-2./1/164	-3.699/63	С	3.565654	-0.096889	1.353929	Н	-1.206183	-3.009438	-0.120212
С	-2.442106	-1.111759	-3.182840	C	4 474707	-1 151674	1 186312	н	0.004360	-4 115765	-1 982913
С	-1.401746	-0.314371	-2.770509	C	4.764264	2.024076	2.240227	11	2 01 49 77	2 712480	2 509625
Н	-2.457604	-1.514620	-4.192060	C	4./04204	-2.024976	2.240227	п	2.0148//	-5./15469	2.308033
C	-2 456555	0 718235	0 7/9125	C	4.149428	-1.859974	3.481535	Н	2.998422	-3.594559	0.326939
č	1 262475	0.506271	1 504260	С	3.240982	-0.812241	3.662109	Н	-0.383854	-3.167464	2.159019
č	-1.303473	0.390271	1.394300	С	2.956042	0.057688	2.611013	Н	4.985521	-1.289342	0.239195
0	-0.228609	-0.112605	1.200020	н	4 387526	-2 527361	4 305073	Н	2 255910	0 872878	2 767716
С	-1.356024	1.101390	2.913764	ц	0.576515	0.064100	3 420427	ц	5 485018	2 824201	2.000277
				11	-0.370313	-0.004199	-3.429427	11	2.465018	-2.024291	2.090277
								п	2.700119	-0.003342	4.028077
			 	C	-3 367623	2 325073	2 486104	н	5 503744	-3 494181	1 328289
			84	C	-3.367623	2.325073	2.486104	Н	5.503744	-3.494181	1.328289
	• a d	L.	X	C C	-3.367623 -3.369557	2.325073 1.821137	2.486104 1.142057	H H	5.503744 4.961676	-3.494181 -1.732933	1.328289 -0.295272
	1.8	A		C C C	-3.367623 -3.369557 -4.393678	2.325073 1.821137 2.274405	2.486104 1.142057 0.265265	H H H	5.503744 4.961676 -0.429525	-3.494181 -1.732933 0.000489	1.328289 -0.295272 -3.427835
	1	$\langle \cdot \rangle$	X	C C C C	-3.367623 -3.369557 -4.393678 -5.372209	2.325073 1.821137 2.274405 3.141840	2.486104 1.142057 0.265265 0.700858	Н Н Н	5.503744 4.961676 -0.429525 -0.442869	-3.494181 -1.732933 0.000489 0.920283	1.328289 -0.295272 -3.427835 3.573966
•		dr.	X	C C C C C C	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224	2.325073 1.821137 2.274405 3.141840 3.602377	2.486104 1.142057 0.265265 0.700858 2.037719	H H H C	5.503744 4.961676 -0.429525 -0.442869 0.774947	-3.494181 -1.732933 0.000489 0.920283 3.254497	1.328289 -0.295272 -3.427835 3.573966 0.918994
•	Å		X	С С С С С С С С С С	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388	H H H C H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357
٩	Ą	×.	Å Å	СССССН	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270	H H H C H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148
~	Å	Ť.	X	C C C C C C H	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 (171100	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.270646	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270	Н Н Н С Н Н	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148
	Ê		X	C C C C C H H	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 2.368000	Н Н Н С Н Н Н	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100
•	Ŕ		X X X	C C C C C H H H	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355	Н Н Н С Н Н Н	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165
	Ŕ		Å Å	C C C C C C H H H H	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169	Н Н Н Н Н Н Н Н Н С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196
	Ŕ	52/c) SN2	X X X	C C C C C C C H H H H H	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914	Н Н Н Н Н Н Н Н Н Н Н Н	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990
	¢¢	S2 _{(R)-SN2p}	X X X	C C C C C C C C H H H H H N	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 -2.136135	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442	H H H C H H H C H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1 947279
°,	¢¢	S2 _{(R)-SN2p}		C C C C C C H H H H H N C	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752	H H H C H H H C H H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508
P	0.855346	S2 _{(R)-SN2p} 0.145139	-0.055152	С С С С С С С Н Н Н Н И О С	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.702717	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453000	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 0.606124	H H H H C H H H H H H H H H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.402817	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775
PO	0.855346 -0.118729	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919}	-0.055152 -1.071604	С С С С С С С Н Н Н Н Н N С С С	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.061002	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184	H H H H H H H H H H H H H H H H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775
P O C	0.855346 -0.118729 -1.282589	S2 _{(R)-SNZP} 0.145139 1.015919 0.346490	-0.055152 -1.071604 -1.477611	C C C C C C H H H H H N C C C C	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020	H H H H H H H H H H H H H H C U	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621
P O C C	0.855346 -0.118729 -1.282589 -2.358648	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427}	-0.055152 -1.071604 -1.477611 -0.610242	С С С С С С С С С С С С С С С С С С С	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228	H H H C H H H H C H H H H C U C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910
P O C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703}	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430	СССССННННИКССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753	H H H H H H H H H H H H H H H C U C U H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209
P O C C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570	S2 _{(R)-SN2P} 0.145139 1.015919 0.346490 0.245427 -0.554703 1.00027(-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 2 272442	С С С С С С С Н Н Н Н Н И О С С С С С С С С С С С С С С С С С С	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.487744 4.242896 4.979315 4.955739	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135	H H H H H H H H H H H H H H H H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078
P O C C C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442	СССССННННИ КСССССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 0.519697	Н Н Н Н С Н Н Н Н С И Н Н Н С И Н Н Н Н	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 2.106694	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404
P O C C C C C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547}	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425	СССССНННН Н NСССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697	H H H H C H H H H C H H H H C C H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.67832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404
P O C C C C C C C C	0.855346 -0.118729 -1.282589 -3.38648 -3.481570 -3.499244 -4.610352 -5.652466	S2 _{(<i>R</i>)-SN2<i>p</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527	СССССНННН Н N ССССССН:	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.453909 3.453909 3.453909 3.453909 3.453909 3.453915 4.955739 4.195336 4.187968	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120	H H H H H H H H H H H H C H H H H C C H H H H C H H H H C H H H H C H H H H C H H H C H H H C H H H C H H H C H H H C H C H C H H C C H C C H C C H C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428
P O C C C C C C C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608}	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999	СССССНННН Н КОСССССНН	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933	H H H H H H H H H H H H H H H C C H H H H C C H H H H C C H H H H C C H H H C C H H H C C H H H C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.794078 -2.842404 0.933428 1.704493
P O C C C C C C C C C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843	S2 _{(R)-SNZP} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712	СССССННННН КОССССССННН	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139	H H H H H H H H H H H H H H H C H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065	$\begin{array}{c} 1.328289\\ -0.295272\\ -3.427835\\ 3.573966\\ 0.918994\\ 0.143357\\ 1.830148\\ 1.134100\\ 1.325165\\ -1.346196\\ -1.773990\\ -1.947279\\ -1.427508\\ 0.471775\\ -0.535621\\ -2.314910\\ -2.272209\\ -2.794078\\ -2.842404\\ 0.933428\\ 1.704493\\ 2.730508\end{array}$
P O C C C C C C C C C H	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854	СССССННННН КССССССНННН	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.453909 3.457744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829	H H H H C H H H H C C H H H H C C H C C H C C H C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292
P O C C C C C C C C C H H	0.855346 0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430041	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596}	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530	СССССНННННИСССССССННННН	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.56769 5.568649 4.262446 2.919021	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139	H H H H H H H H H H H H C H H H H C C H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.67832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552
P O C C C C C C C C H H H	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 (4052)	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 2.20225	СОСССНННННИОСССССНННННО	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597303	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -2.098139 0.114587	H H H H C H H H H C C H H H C C H C C C C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.2842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631
P OC C C C C C C C H H H	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135	ОССССННННН И ОССССССНННННОС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.1955336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 0.582300	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767	H H H H C H H H H C C H H H C C H C C C C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 0.222051	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 4.204985 -4.20485 -4.20485	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 0.930572
РОССССССС Н Н Н Н	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346	СССССНННННКСССССССНННННССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 -0.722222	H H H H C H H H H C C H H H H C C C C C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.695467 -2.695467	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573
Р ОСССССССС Н Н Н Н Н С	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.81138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514	ООСОСННННН И ОСОСОСОНННННООО	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289	H H H H C H H H H C C H H H C C H C C C C C H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.67832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283
РОССССССС Н Н Н Н С С	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.430941 -6.430941 -6.430941 -6.430941 -2.395413 -1.290097	S2(R)-SN2p 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057	СССССНННННИОССССССНННННСССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993	H H H H C H H H H C C H H H C C C C C C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678322 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474 -4.183787	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399
РОССССССССННННССН	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106	S2 (<i>R</i>)- SN2 <i>P</i> 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759	СССССНННННКОССССССННННССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958 4.364082	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.587393 -0.583399 -1.671078 -2.673222 -2.608964	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060	Н Н Н Н С Н Н Н Н С С Н Н Н Н С С С С С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424855 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474 -4.183787 -2.802022	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673
РОССССССССННННССНС	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919290	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957	ССССССНННННКОССССССНННННОССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.52745 4.857958 4.364082 3.550386	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 -2.608964 -1.533414	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224	Н Н Н Н С Н Н Н Н С И Н Н Н С С Н С С С С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183 -0.342073	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474 -4.183787 -2.802022 -4.814468	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673 -1.902177
РОССССССССННННССНСС	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774	S2 _{(<i>P</i>)-SN2<i>p</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919280 0.755162	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957	СССССНННННИССССССНННННОСССССС	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958 4.364082 3.550386 3.242006	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 -2.608964 -1.533414 -0.533735	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224 2.382243	Н Н Н Н С Н Н Н Н С С Н Н И С С И С С С С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678322 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.426496 1.426496 1.426496 1.426496 1.426496 1.426496 1.426496 1.426496 1.426496 1.426495 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183 -0.342073 -0.330620	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474 -4.183787 -2.802022 -4.814468 -5.703593	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673 -1.902177 -0.38554
P O C C C C C C C C H H H H H C C H C C C	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774 -1.270684	S2 _{(<i>R</i>)-SN2_{<i>P</i>} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919280 0.705192}	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957 1.596174	СССССНННННИССССССНННННССССССЧ	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.33373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958 4.364082 3.50386 3.242096 3.242096	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.56769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 2.608964 -1.533414 -0.533735	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224 2.382243	H H H H C H H H H C C H H H H C C C C C	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.67832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183 -0.330629	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673 -1.902177 -0.386554
РОССССССССННННССНССО	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774 -1.270684 -0.171689	S2 (<i>R</i>)- SN2 <i>P</i> 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919280 0.705192 -0.077440	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957 1.596174 1.237296	ОССССИННННИ ИСССССССИННННОСССССИ:	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958 4.364082 3.550386 3.242096 2.619357 2.17202	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 -2.608964 -1.533414 -0.533735 0.301526	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224 2.382243 2.688378	Н Н Н Н С Н Н Н Н С И Н Н Н И С С Н Н С С С С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183 -0.342073 -0.330629 -1.786334	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.695467 -3.650474 -4.183787 -2.802022 -4.814468 -5.703593 -2.718868 -2.718868 -4.405467 -2.802022 -4.814468 -5.703593 -2.718868 -2.718887 -2.718887 -2.718887 -2.7187 -2.7187 -2.7187 -2.7187 -2.7187 -2.7187	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 2.274078 2.2842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673 -1.902177 -0.386554 1.590503
РОССССССССННННССНССОС	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774 -1.270684 -0.171689 -1.272956	S2 _{(R)-SNZP} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919280 0.705192 -0.077440 1.183220	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957 1.596174 1.237296 2.926122	ОСССССННННН И ОССССССНННННССССССНН.	-3.367623 -3.369557 -4.393678 -5.372209 -5.389224 -4.401996 -4.388787 -6.171100 -6.135683 -4.394637 -2.333373 2.116135 2.121099 2.703717 2.064093 2.595153 3.769254 4.409241 3.878080 4.379625 5.320050 4.178719 2.089481 1.151689 3.498168 3.731906 4.542745 4.857958 4.364082 3.550386 3.242096 2.619357 3.171382	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.487744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 -2.608964 -1.533414 -0.533735 0.301526 -1.464164	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224 2.382243 2.688378 4.319248	Н Н Н Н С Н Н Н Н С И Н Н Н С С Н С С С С	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.424885 1.304904 0.227207 0.400992 -1.195845 -1.330948 1.155406 -0.232951 2.306518 -2.319098 -1.273183 -0.342073 -0.330629 -1.786334 -1.612318	-3.494181 -1.732933 0.000489 0.920283 3.254497 3.175878 2.777676 4.317001 2.802331 0.340226 -0.510752 1.224555 0.136638 1.403817 -2.092094 -2.988936 -2.996398 -3.885887 -2.106694 -3.736063 -3.421961 -3.105065 -3.581595 -3.780136 -4.204985 -4.204985 -4.204985 -4.204985 -4.695467 -3.650474 -4.183787 -2.802022 -4.814468 -5.703593 -2.718686 -4.445354	1.328289 -0.295272 -3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 -1.346196 -1.773990 -1.947279 -1.427508 0.471775 -0.535621 -2.314910 -2.272209 -2.794078 -2.842404 0.933428 1.704493 2.730508 1.259292 -0.259552 -0.454631 -0.820573 1.348283 -0.500399 -0.757673 -1.902177 -0.386554 1.590503 1.803071
РОСССССССС ННННССНССОСС	0.855346 -0.118729 -1.282589 -2.358648 -3.481570 -3.499244 -4.610352 -5.652466 -5.618151 -4.565843 -4.559739 -6.430941 -6.495012 -4.615287 -2.395413 -1.290097 -2.429106 -2.323774 -1.270684 -0.171689 -1.272956 -2.316533	S2 _{(R)-SN2p} 0.145139 1.015919 0.346490 0.245427 -0.554703 -1.090276 -1.866547 -2.142126 -1.654608 -0.881138 -0.517899 -1.891596 -2.738848 -2.247969 -0.858507 -0.176222 -1.244539 0.919280 0.705192 -0.077440 1.183220 1.957150	-0.055152 -1.071604 -1.477611 -0.610242 -1.039430 -2.372442 -2.800425 -1.945527 -0.617999 -0.177712 0.842854 0.062530 -2.282135 -3.818346 -3.236514 -2.790057 -4.251759 0.718957 1.596174 1.237296 2.926122 3.367469	О О О О О О Н Н Н Н Н И О О О О О О О Н Н Н Н	$\begin{array}{c} -3.367623\\ -3.369557\\ -4.393678\\ -5.372209\\ -5.389224\\ -4.401996\\ -4.388787\\ -6.171100\\ -6.135683\\ -4.394637\\ -2.333373\\ 2.116135\\ 2.121099\\ 2.703717\\ 2.064093\\ 2.595153\\ 3.769254\\ 4.409241\\ 3.878080\\ 4.379625\\ 5.320050\\ 4.178719\\ 2.089481\\ 1.151689\\ 3.498168\\ 3.731906\\ 4.542745\\ 4.857958\\ 4.364082\\ 3.550386\\ 3.242096\\ 2.619357\\ 3.171382\\ 4.619955\end{array}$	2.325073 1.821137 2.274405 3.141840 3.602377 3.202410 3.564299 4.279646 3.480411 1.945313 2.321857 1.185487 2.675030 3.453909 3.453909 3.45744 4.242896 4.979315 4.955739 4.195336 4.187968 5.526769 5.568649 4.262446 2.919021 0.597393 -0.583399 -1.671078 -2.673222 -2.608964 -1.533414 -0.533735 0.301526 -1.464164 -3.378586	2.486104 1.142057 0.265265 0.700858 2.037719 2.908388 3.933270 2.368000 0.006355 -0.767169 4.390914 0.235442 0.479752 -0.696184 -1.945020 -2.990228 -2.803753 -1.565135 -0.519697 0.446120 -1.408933 -3.619139 -3.951829 -2.098139 0.114587 1.064767 0.703289 1.627993 2.931060 3.303224 2.382243 2.688378 4.319248 3.653635	H H H H C H H H H C H H H H H H H H H H	5.503744 4.961676 -0.429525 -0.442869 0.774947 0.011349 0.407477 0.923508 2.809180 3.896312 3.354964 3.678832 4.968672 4.148277 1.290679 1.806039 2.896642 1.426496 1.426666 1.426666 1.426666 1.426666 1.426666 1.426666 1.426666 1.426666 1.42666666666666666666666666666666666666	$\begin{array}{c} -3.494181\\ -1.732933\\ 0.000489\\ 0.920283\\ 3.254497\\ 3.175878\\ 2.777676\\ 4.317001\\ 2.802331\\ 0.340226\\ -0.510752\\ 1.224555\\ 0.136638\\ 1.403817\\ -2.092094\\ -2.988936\\ -2.996398\\ -3.885887\\ -2.106694\\ -3.736063\\ -3.421961\\ -3.105065\\ -3.581595\\ -3.780136\\ -4.204985\\ -4.695467\\ -3.650474\\ -4.183787\\ -2.802022\\ -4.814468\\ -5.703593\\ -2.718686\\ -4.445354\\ -4.809302\\ \end{array}$	1.328289 - 0.295272 - 3.427835 3.573966 0.918994 0.143357 1.830148 1.134100 1.325165 - 1.346196 - 1.773990 - 1.947279 - 1.427508 0.471775 - 0.535621 - 2.314910 - 2.272209 - 2.794078 - 2.842404 0.933428 1.704493 2.730508 1.259292 - 0.259552 - 0.454631 - 0.820573 1.348283 - 0.500399 - 0.757673 - 1.902177 - 0.386554 1.590503 1.803071 - 0.809367

	C	3.661326	-2.525357	2.186953	Н	-5.351541	3.014229	1.888303
	С	3.579862	-1.814371	0.942873	Н	-4.863735	1.421906	0.080224
It Y M	č	4 613826	-2 025476	-0.010840	н	0 382946	0 414928	-3 248173
VI See M		5 677262	2 858011	0.264057	и П	0.650847	1 591955	2 522220
- INTER	C C	5.077205	-2.636011	0.204037	п С	0.039847	-1.381855	3.333220
	S _P C	5.773935	-3.523065	1.508259	C	-0.523448	-3.541251	0.5/8/8/
	C C	4.780901	-3.360391	2.446365	Н	0.215800	-3.298681	-0.186879
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	Н	6.622115	-4.169441	1.712991	Н	-0.598426	-4.631272	0.635105
• I 9 • -	н	6 447110	-3.009503	-0.487142	н	-2 573514	-3 281/11	1.074625
с С	0 II II	4 556020	1 526420	0.076077	C	2.973314	0.522509	1.109442
C2 _{(R)-SN2p}	п	4.556050	-1.330429	-0.9/60//	U U	-5.842029	-0.332398	-1.198442
	Н	2.687551	-2.920792	4.082532	Н	-3.335200	0.380076	-1.538212
P -0 791585 -0 345763 0 0	090089 N	-1.988686	-1.486176	0.226297	Н	-3.611285	-1.331045	-1.905036
0 0 206333 -0 960471 -1 0	069547 C	-1.912519	-2.990784	0.247952	Н	-4.921668	-0.355083	-1.231336
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C 3.426204 0.873392 -0.8	827942 C	-2.508457	-4.070343	-3.403844	U U	-1.5/5942	3./11214	-2.318802
C 3.370510 1.601068 -2.0	065266 C	-3.5018/9	-4.884523	-3.314/12	н	-2.35/849	3.2/0/62	-2./22618
C 4.402893 2.525862 -2.3	380281 C	-4.120644	-5.069998	-2.079004	Н	-1.063312	4.256981	-3.416165
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C = 5.467650 = 2.081015 = 0.2000	260615 H	-4.092214	-4.597786	0.021278	С	-2.055173	3.997728	-0.094977
C 14042(5 11(1727 0.0	200013 H	-4 999479	-5 703150	-1 996570	С	-1 414495	3 793500	1 095524
C 4.494365 1.161/2/ 0.0	J6624/ H	3 896020	5 371040	4 201760	й	2 002182	3 173386	1 058830
H 4.536440 0.654864 1.0	)22746 11	-3.890020	-3.371949	4.201700	п С	-2.002182	4 1575(5	1.217220
Н 6.269265 2.286274 0.4	442993 п	-1.8/8920	-3.92/391	-4.303312	Č	0.055012	4.13/303	1.51/520
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H 4355189 3053565 -33	329512 C	-3.393900	-0.943505	0.212049	С	-1.420039	4.658732	-1.303884
C = 2.273559 = 1.404068 = 2.9	946475 C	-3.621207	0.124991	1.290796	С	-0.040900	5.265207	-0.951910
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	599088 -	-4 710245	2 160131	2 088585	н	1 757992	4 819323	0 183141
H 2.253242 1.938550 -3.8	892372 C	4 106222	1 054678	2 269257	и П	0.060000	2 207642	0.100141
C 2.447124 -0.955614 0.6	686899 C	-4.190333	1.934078	3.308337		0.909990	5.397043	-0.480329
C 1.407099 -0.981932 1.6	603394 C	-3.395/10	0.833659	3.614511	Н	0.51/2//	5.461143	-1.8/4219
O 0.229566 -0.258239 1.3	391854 C	-3.116453	-0.069412	2.590908	Н	-0.194304	6.238373	-0.467381
C 1 488871 -1 663962 2.8	837782 H	-2.502933	-0.940560	2.799439	Н	0.525359	3.392940	1.931406
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C 2.008423 -2.400913 5.1	Н	-4 428929	2 648481	4 170965	н	-2.096668	5 482919	-1 573100
			2.010101			2.070000	0.102/1/	1.070100
9	С	3.156303	1.978962	3.244224	С	3.875753	-1.075961	0.515803
	Č	3 563037	2 987431	2 330244	Ĥ	3 750140	-0.321122	-0.260623
~ ?*	C	2.025916	2.069075	1.047040	11	2 504402	0.646924	1 476022
14 840	C	2.923610	3.008073	1.04/049	11	3.364463	-0.040824	1.4/0923
	( ·	3.4111/8	4.040449	11 1 / X 1 1 6	н	4.9386/4	-1.3338/8	0.369494
	C			0.120110	11			
	C	4.434357	4.898670	0.468338	Н	3.323031	-3.048286	1.046528
Star L	C C C	4.434357 5.030782	4.898670 4.840933	0.468338	H C	3.323031 0.421141	-3.048286 -4.150918	1.046528 -0.948637
		4.434357 5.030782 4.602069	4.898670 4.840933 3.899290	0.468338 1.749322 2.656515	H C H	3.323031 0.421141 -0.384801	-3.048286 -4.150918 -3.553714	1.046528 -0.948637 -1.384426
		4.434357 5.030782 4.602069 5.063520	4.898670 4.840933 3.899290 3.827683	0.468338 1.749322 2.656515 3.638684	H C H H	3.323031 0.421141 -0.384801 1.249282	-3.048286 -4.150918 -3.553714 -4.180079	1.046528 -0.948637 -1.384426 -1.659088
	СССНН	4.434357 5.030782 4.602069 5.063520 5.831487	4.898670 4.840933 3.899290 3.827683 5.528322	0.468338 1.749322 2.656515 3.638684 2.007363	H C H H	3.323031 0.421141 -0.384801 1.249282 0.061592	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328	1.046528 -0.948637 -1.384426 -1.659088 -0.805816
	СССНН	4.434357 5.030782 4.602069 5.063520 5.831487 4.780828	4.898670 4.840933 3.899290 3.827683 5.528322	0.468338 1.749322 2.656515 3.638684 2.007363 0.258700	H C H H H	3.323031 0.421141 -0.384801 1.249282 0.061592	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328	1.046528 -0.948637 -1.384426 -1.659088 -0.805816
A A	СССННН	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.904457	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709	H C H H H H	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993
	СССННН	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457	0.123110 0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432	H C H H H H Cu	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275
C1 _{(R)-SN2}	СССННННН	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053	0.123110 0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834	H C H H H Cu C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898
C1 _{(R)-SN2}	СССННННИ	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621	H C H H H C U C H	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0	C C C C H H H H H H H H N 0006702 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359	H C H H H C U C H H	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138
С1 _{(R)-SN2} Р 0.597986 -0.913254 0.0 О 1.522046 -0.013874 -10	C C C C H H H H H H H H N 0006702 C 0065065 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564	H C H H H C U C H H H H	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.904764 -1 459304	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343
Р 0.597986 -0.913254 0.0 0 1.522046 -0.013874 -1.0 0 0.945626 1.210324 -1.4	C C C C H H H H H H H H H N 0006702 C 065065 C C 402986 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433901	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545	H C H H H C U C H H H C U C H H H C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.904764 -1.459304 -3.283778	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295
P 0.597986 -0.913254 0.0 0 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 0.945626 1.210324 -1.4	C C C C H H H H H H H H N 0006702 C 0065065 C 402986 C C 402986 C C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 2.057674	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 2.458225	H H H H H C H H H C H H H C H H H C H H H C H H H C C H H H C H H H C C H H H H C C H H H H C C H H H H C C H H H H C C C C H H H C C C C C C C C C C C C C C C C C C C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.630651	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.4526600
P 0.597986 -0.913254 0.0 0 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5	C C C C C H H H H H H H H H H N 0006702 C 0065065 C 402986 C 537519 C C 0052605 C 402986 C 537519 C C C C C C C C C C C C C C C C C C C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259	4.898670 4.840933 3.899290 3.827683 5.528322 5.628313 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225	H C H H H H C U C H H H C C H H H C C C H H H C C C H H H C C C H H H C C C H H H H C C C C C C C C C C C C C C C C C C C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 0.2020202\end{array}$
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0 O 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5 C 0.361988 3.499090 -0.8	C C C C H H H H H H H H H N N 006702 C 065065 C 402986 C 537519 C 876387 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543	H H H H H C U H H H C C C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0 O 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5 C 0.361988 3.499090 -0.8 C -0.325943 3.586692 -2.	C C C C H H H H H H H H H H O006702 C 065065 C 402986 C 537519 C 876387 C 134190 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375	H H H H H H C H H H C C H H H C C C C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.89394 -3.283778 -2.509885 -2.829439 -4.541490	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341
Р 0.597986 -0.913254 0.0 0 1.522046 -0.013874 -1.1 С 0.945626 1.210324 -1.4 С 1.068034 2.286933 -0.5 С 0.361988 3.499090 -0.8 С -0.325943 3.586692 -2. С -1.013553 4.783197 -2.4	C C C C C H H H H H H H H H H H N 0006702 C 0065065 C 402986 C 537519 C 8376387 C 134190 C 473864 C C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949	H H H H H H C H H H C C H H H C C C C C	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -0.447295 0.659690 2.002883 -0.434341 -1.358325
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0 O 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5 C 0.361988 3.499090 -0.8 C -0.325943 3.586692 -2. C -1.013553 4.783197 -2.4 C -1.059249 5.846911 -1.0	C C C C C H H H H H H H H H N 0006702 C 065065 C 402986 C 537519 C 876387 C 134190 C 473864 C 602927 H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 4.209756 -4.664544	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.352543 -2.098375 -0.958949 0.016602	н Н С Н Н Н Н С С С Н Н Н С С С С Н С	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669
$\begin{array}{c} \hline \\ \hline $	C C C C C H H H H H H H H H H H N 0006702 C 0065065 C 402986 C 537519 C 876387 C 134190 C 473864 C 602927 H 344390 H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485605	4.898670 4.840933 3.899290 3.827683 5.528322 5.62813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496	н Н С Н Н Н Н С С Н Н Н С С С С Н С С	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0 O 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5 C 0.361988 3.499090 -0.8 C -0.325943 3.586692 -2.1 C -1.013553 4.783197 -2.4 C -1.059249 5.846911 -1.0 C -0.421343 5.748860 -0.0 C -0.260826 4.610282 -0.0	C C C C H H H H H H H H H H N N 0006702 C 0065065 C 402986 C 537519 C 876387 C 134190 C 473864 C 602927 H 344390 H 344390 H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865	4.898670 4.840933 3.899290 3.827683 5.528322 5.62813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 74 4705182	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202	н Н С Н Н Н Н С С С С Н С С Н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653
C1 _{(R)-SN2} P 0.597986 -0.913254 0.0 O 1.522046 -0.013874 -1.0 C 0.945626 1.210324 -1.4 C 1.068034 2.286933 -0.5 C 0.361988 3.499090 -0.8 C -0.325943 3.586692 -2. C -1.013553 4.783197 -2.4 C -1.059249 5.846911 -1.0 C -0.421343 5.748860 -0.0 C 0.269826 4.610282 0.0 C 0.269826 4.610282 0.0 C 0.269826 4.610282 0.0	C C C C H H H H H H H H H H H H H M O006702 C 0065065 C 402986 C 537519 C 876387 C 134190 C 473864 C 602927 H 344390 H 008296 H 008296 H 008296 H 008296 H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 2.604550	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 4.432482	H C H H H H C C C H H H C C C C H C C H U	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.89394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 2-4.958682 5 706620	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.872262
$\begin{array}{c} \hline \\ \hline $	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.008652	н н с н н н с с н н н с с с с с с с н с н н н с с н н н с с с с с н с с с с с с	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 -1.607200	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.870262 0.612202
$\begin{array}{c} \hline \\ \hline $	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798	4.898670 4.840933 3.899290 3.827683 5.528322 5.628313 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908	н с н н н н с с с н с с н н н н т.	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -9.5706630 -1.666510	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ \end{array}$
$\begin{array}{c} \hline c1_{(R)-SN2} \\ \hline P & 0.597986 & -0.913254 & 0.0 \\ O & 1.522046 & -0.013874 & -1.1 \\ C & 0.945626 & 1.210324 & -1.4 \\ C & 1.068034 & 2.286933 & -0.5 \\ C & 0.361988 & 3.499090 & -0.8 \\ C & -0.325943 & 3.586692 & -2. \\ C & -1.013553 & 4.783197 & -2.4 \\ C & -1.059249 & 5.846911 & -1.1 \\ C & -0.421343 & 5.748860 & -0.3 \\ C & 0.269826 & 4.610282 & 0.0 \\ H & 0.742047 & 4.552096 & 0.5 \\ H & -0.481927 & 6.577692 & 0.3 \\ H & -1.595771 & 6.752789 & -1.3 \\ \end{array}$	C C C C C H H H H H H H H H H H H N N 006702 C 065065 C 402986 C 537519 C 876387 C 134190 C 473864 C 6602927 H 344390 H 344390 H 344390 H 981572 H 355614 H 870557 C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562	$\begin{array}{r} 4.898670\\ 4.840933\\ 3.899290\\ 3.827683\\ 5.528322\\ 5.62813\\ 4.094457\\ 1.937053\\ -2.241655\\ -2.363895\\ -3.027887\\ -2.455610\\ -3.057674\\ -4.238049\\ -4.813008\\ -4.209756\\ -4.664544\\ -5.731777\\ -4.705182\\ -2.604050\\ -1.541921\\ -3.568247\\ \end{array}$	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272	н с н н н н с с с н н н с с с с н с с н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506	$\begin{array}{r} -3.048286\\ -4.150918\\ -3.553714\\ -4.180079\\ -5.176328\\ -4.232875\\ -1.068930\\ -2.041595\\ -2.914821\\ -1.388607\\ -2.408199\\ 0.470683\\ 0.639671\\ 0.023083\\ -0.338127\\ -0.896858\\ -1.221033\\ -0.479129\\ 0.372308\\ -1.607200\\ 1.322600\\ 1.045794 \end{array}$	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\end{array}$
$\begin{array}{c} \hline c1_{(R)-SN2} \\ \hline c1_{(R)-SN2} \\$	C C C C C H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.428625 5.123865 5.123865 5.123865 2.854798 0.904562 -0.154672	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735	н с н н н н с ^и с н н н с с с с с н с с н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -5.706630 -1.666510 -3.081506 -4.403466	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\end{array}$
$\begin{array}{c} \hline \\ \hline $	C C C C C H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473 -4.005311	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396	н с н н н н с с с н с с н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.322600 1.045794 -1.135275 -2.083892	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.870262 0.610303 -1.347141 2.950765 0.650567
$\begin{array}{c} \hline \\ P & 0.597986 & -0.913254 & 0.0\\ O & 1.522046 & -0.013874 & -1.0\\ C & 0.945626 & 1.210324 & -1.4\\ C & 1.068034 & 2.286933 & -0.5\\ C & 0.361988 & 3.499090 & -0.8\\ C & -0.325943 & 3.586692 & -2.\\ C & -1.013553 & 4.783197 & -2.4\\ C & 1.059249 & 5.846911 & -1.0\\ C & -0.421343 & 5.748860 & -0.5\\ C & 0.269826 & 4.610282 & 0.0\\ H & 0.742047 & 4.552096 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -1.519530 & 4.833544 & -3.4\\ C & -0.337627 & 2.465083 & -3.0\\ C & 0.262276 & 1.285881 & -2.6\\ \end{array}$	C C C C C H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473 -4.005311 -4.043651	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622	н с н н н н с с с н с с н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275 -2.083892 -0.796959	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.870262 0.610303 -1.347141 2.950765 0.650567 2.211943
$\begin{array}{c} \label{eq:result} \\ P & 0.597986 & -0.913254 & 0.0\\ 0 & 1.522046 & -0.013874 & -1.0\\ C & 0.945626 & 1.210324 & -1.4\\ C & 1.068034 & 2.286933 & -0.5\\ C & 0.361988 & 3.499090 & -0.8\\ C & -0.325943 & 3.586692 & -2.\\ C & -1.013553 & 4.783197 & -2.\\ C & -1.059249 & 5.846911 & -1.0\\ C & -0.421343 & 5.748860 & -0.5\\ C & 0.269826 & 4.610282 & 0.0\\ H & 0.742047 & 4.552096 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -1.595771 & 6.752789 & -1.3\\ H & -1.519530 & 4.833544 & -3.4\\ C & -0.337627 & 2.465083 & -3.0\\ C & 0.262276 & 1.285881 & -2.0\\ H & -0.855266 & 2.542218 & -2.5\\ \end{array}$	C C C C C C C C C C C C C C C C C C C	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.98155	$\begin{array}{r} 4.898670\\ 4.840933\\ 3.899290\\ 3.827683\\ 5.528322\\ 5.62813\\ 4.094457\\ 1.937053\\ -2.241655\\ -2.363895\\ -3.027887\\ -2.455610\\ -3.057674\\ -4.238049\\ -4.813008\\ -4.209756\\ -4.664544\\ -5.731777\\ -4.705182\\ -2.604050\\ -1.541921\\ -3.568247\\ -3.539473\\ -4.005311\\ -4.043651\\ -3.613308\end{array}$	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267	н с н н н н с с н н н с с с с с н с с н н н н н н н н н н н н н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.76669	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275 -2.083892 -0.796959 -4.343395	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.870262 0.610303 -1.347141 2.950765 0.650567 2.211943 0.315841
$\begin{array}{c} \label{eq:constraint} \hline \\ \end{cases} \\ \end{cases}$	C C C C C C C H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155	4.898670 4.840933 3.899290 3.827683 5.528322 5.62813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473 -4.005311 -4.043651 -3.613398 -3.14104	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 2.855622	нсннннсоснннсоссноснннннннн н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.89394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275 -2.083892 -0.796959 -4.343395 -2.706625	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\\ 0.650567\\ 2.211943\\ 0.315841\\ 0.315841\\ 0.315841\\ \end{array}$
$\begin{array}{c} \hline \\ \hline $	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.428625 5.123865 5.885376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155 -0.698334	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.209756 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473 -4.005311 -4.043651 -3.613398 -3.141104	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 3.835231	: Н С Н Н Н Н С С Н Н Н С С С С Н Н С И Н Н Н Н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699 1.218805	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275 -2.083892 -0.796959 -4.343395 -2.7406720	1.046528 -0.948637 -1.384426 -1.659088 -0.805816 0.751993 -0.915275 -2.520898 -2.247764 -3.145138 -3.157343 -0.447295 0.659690 2.002883 -0.434341 -1.358325 0.801669 2.081513 2.220653 0.870262 0.610303 -1.347141 2.950765 0.650567 2.211943 0.315841 2.949757
$\begin{array}{c} \label{eq:result} \\ P & 0.597986 & -0.913254 & 0.0\\ O & 1.522046 & -0.013874 & -1.0\\ O & 1.522046 & -0.013874 & -1.4\\ C & 0.945626 & 1.210324 & -1.4\\ C & 1.068034 & 2.286933 & -0.5\\ C & 0.361988 & 3.499090 & -0.8\\ C & -0.325943 & 3.586692 & -2.\\ C & -1.013553 & 4.783197 & -2.4\\ C & 1.059249 & 5.846911 & -1.0\\ C & -0.421343 & 5.748860 & -0.3\\ C & 0.269826 & 4.610282 & 0.0\\ H & 0.742047 & 4.552096 & 0.5\\ H & -0.481927 & 6.577692 & 0.3\\ H & -1.595771 & 6.752789 & -1.3\\ H & -1.519530 & 4.833544 & -3.3\\ C & -0.337627 & 2.465083 & -3.0\\ C & 0.262276 & 1.285881 & -2.6\\ H & -0.855266 & 2.542218 & -3.3\\ C & 1.862104 & 2.150819 & 0.7\\ C & 1.602423 & 1.114267 & 1.6\\ \end{array}$	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155 -0.698334 0.210238	4.898670 4.840933 3.899290 3.827683 5.528322 5.623813 4.094457 1.937053 -2.241655 -2.363895 -3.027887 -2.455610 -3.057674 -4.238049 -4.813008 -4.203766 -4.664544 -5.731777 -4.705182 -2.604050 -1.541921 -3.568247 -3.539473 -4.043651 -3.613398 -3.141104 -3.108844	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.458225 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 3.835231 2.779548	н с н н н н с с с с с с с с н с с н н н н н н н н н н н н н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699 1.218805 -3.380418	$\begin{array}{r} -3.048286\\ -4.150918\\ -3.553714\\ -4.180079\\ -5.176328\\ -4.232875\\ -1.068930\\ -2.041595\\ -2.914821\\ -1.388607\\ -2.408199\\ 0.470683\\ 0.639671\\ 0.023083\\ -0.338127\\ -0.896858\\ -1.221033\\ -0.372308\\ -1.607200\\ 1.322600\\ 1.045794\\ -1.135275\\ -2.083892\\ -0.796959\\ -4.343395\\ -2.740683\\ -4.415785\end{array}$	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.81513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\\ 0.650567\\ 2.211943\\ 0.315841\\ 2.949757\\ 2.180985\\ \end{array}$
$\begin{array}{c} \label{eq:result} \\ P & 0.597986 & -0.913254 & 0.0\\ O & 1.522046 & -0.013874 & -1.0\\ C & 0.945626 & 1.210324 & -1.4\\ C & 1.068034 & 2.286933 & -0.5\\ C & 0.361988 & 3.499090 & -0.8\\ C & -0.325943 & 3.586692 & -2.\\ C & -1.013553 & 4.783197 & -2.\\ C & -1.059249 & 5.846911 & -1.0\\ C & -0.421343 & 5.748860 & -0.0\\ C & -0.421343 & 5.748860 & -0.0\\ C & 0.269826 & 4.610282 & 0.0\\ H & 0.742047 & 4.552096 & 0.5\\ H & -0.481927 & 6.577692 & 0.3\\ H & -1.595771 & 6.752789 & -1.3\\ H & -0.855266 & 2.542218 & -3.0\\ C & 0.262276 & 1.285881 & -2.6\\ H & -0.855266 & 2.542218 & -3.5\\ C & 1.862104 & 2.150819 & 0.7\\ C & 1.602423 & 1.114267 & 1.6\\ O & 0.673145 & 0.131761 & 1.3\\ \end{array}$	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.97258 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155 -0.698334 0.210238 -2.706547	$\begin{array}{r} 4.898670\\ 4.840933\\ 3.899290\\ 3.827683\\ 5.528322\\ 5.62813\\ 4.094457\\ 1.937053\\ -2.241655\\ -2.363895\\ -3.027887\\ -2.455610\\ -3.057674\\ -4.238049\\ -4.813008\\ -4.209756\\ -4.664544\\ -5.731777\\ -4.705182\\ -2.604050\\ -1.541921\\ -3.568247\\ -3.59473\\ -4.005311\\ -4.043651\\ -3.613398\\ -3.141104\\ -3.108844\\ -3.108844\\ -3.648183\end{array}$	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 3.835231 2.779548 4.450543	н н с н н н н с с с н н н с с с с н с с н н н н н н н н н н н н н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.276934 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.685176 -4.281362 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699 1.218805 -3.380418 -0.391566	$\begin{array}{r} -3.048286\\ -4.150918\\ -3.553714\\ -4.180079\\ -5.176328\\ -4.232875\\ -1.068930\\ -2.041595\\ -2.914821\\ -1.388607\\ -2.408199\\ 0.470683\\ 0.639671\\ 0.023083\\ -0.338127\\ -0.896858\\ -1.221033\\ -0.372108\\ -1.607200\\ 1.322600\\ 1.045794\\ -1.135275\\ -2.083892\\ -0.796959\\ -4.343395\\ -2.740683\\ -4.415785\\ -2.805590\end{array}$	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\\ 0.650567\\ 2.211943\\ 0.315841\\ 2.949757\\ 2.180985\\ 4.822501\end{array}$
$\begin{array}{c} \label{eq:constraints} \\ P & 0.597986 & -0.913254 & 0.0\\ 0 & 1.522046 & -0.013874 & -1.0\\ C & 0.945626 & 1.210324 & -1.4\\ C & 1.068034 & 2.286933 & -0.5\\ C & 0.361988 & 3.499090 & -0.8\\ C & -0.325943 & 3.586692 & -2.\\ C & -1.013553 & 4.783197 & -2.4\\ C & -1.059249 & 5.846911 & -1.6\\ C & -0.421343 & 5.748860 & -0.5\\ C & -0.421343 & 5.748860 & -0.5\\ C & 0.269826 & 4.610282 & 0.0\\ H & 0.742047 & 4.552096 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -0.481927 & 6.577692 & 0.5\\ H & -1.595771 & 6.752789 & -1.3\\ H & -1.519530 & 4.833544 & -3.4\\ C & -0.337627 & 2.465083 & -3.6\\ C & 0.262276 & 1.285881 & -2.6\\ H & -0.855266 & 2.542218 & -3.5\\ C & 1.862104 & 2.150819 & 0.7\\ C & 1.602423 & 1.114267 & 1.6\\ O & 0.673145 & 0.131761 & 1.3\\ C & 2.216105 & 1.048782 & 2.8\\ \end{array}$	C C C C H H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155 -0.698334 0.210238 -2.706547 0.227599	$\begin{array}{r} 4.898670\\ 4.840933\\ 3.899290\\ 3.827683\\ 5.528322\\ 5.62813\\ 4.094457\\ 1.937053\\ -2.241655\\ -2.363895\\ -3.027887\\ -2.455610\\ -3.057674\\ -4.238049\\ -4.813008\\ -4.209756\\ -4.664544\\ -5.731777\\ -4.705182\\ -2.604050\\ -1.541921\\ -3.568247\\ -3.539473\\ -4.005311\\ -4.043651\\ -3.613398\\ -3.141104\\ -3.108844\\ -3.648183\\ 0.404147\end{array}$	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.226621 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.242202 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 3.835231 2.779548 4.450543 -3.268800	¹ Н С Н Н Н Н ² С Н Н Н С С С С Н С С Н Н Н Н Н Н Н Н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699 1.218805 -3.380418 -0.391566 -2.645281	$\begin{array}{r} -3.048286\\ -4.150918\\ -3.553714\\ -4.180079\\ -5.176328\\ -4.232875\\ -1.068930\\ -2.041595\\ -2.914821\\ -1.388607\\ -2.408199\\ 0.470683\\ 0.639671\\ 0.023083\\ -0.338127\\ -0.896858\\ -1.221033\\ -0.479129\\ 0.372308\\ -1.607200\\ 1.322600\\ 1.045794\\ -1.135275\\ -2.083892\\ -0.796959\\ -2.740683\\ -4.415785\\ -2.805590\\ 0.771232\end{array}$	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.0816513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\\ 0.650567\\ 2.211943\\ 0.315841\\ 2.949757\\ 2.180985\\ 4.822501\\ 2.785069\end{array}$
$\begin{array}{c} \hline \\ \hline $	C C C C C H H H H H H H H H H H H H H H	4.434357 5.030782 4.602069 5.063520 5.831487 4.789838 2.974960 3.621696 1.604502 3.099083 3.629347 3.433991 3.968259 4.710148 4.912758 4.373417 4.535495 5.485625 5.123865 3.805376 2.854798 0.904562 -0.154672 -1.461095 -2.374343 -1.998155 -0.698334 0.210238 2.706547 0.227599 1.912469	$\begin{array}{r} 4.898670\\ 4.840933\\ 3.899290\\ 3.827683\\ 5.528322\\ 5.62813\\ 4.094457\\ 1.937053\\ -2.241655\\ -2.363895\\ -3.027887\\ -2.455610\\ -3.057674\\ -4.238049\\ -4.813008\\ -4.209756\\ -4.664544\\ -5.731777\\ -4.705182\\ -2.604050\\ -1.541921\\ -3.568247\\ -3.539473\\ -4.0053111\\ -4.043651\\ -3.613398\\ -3.141104\\ -3.108844\\ -3.648183\\ 0.404147\\ 0.250676\end{array}$	0.468338 1.749322 2.656515 3.638684 2.007363 -0.258709 -0.862432 4.225834 0.217359 -1.053564 -2.319545 -3.458225 -3.352543 -2.098375 -0.958949 0.016602 -2.003496 -4.432483 -2.408908 0.385272 1.492735 1.296396 2.355622 3.627267 3.835231 2.779548 4.450543 -3.268800 3.552174	н н с н н н н с с с н н н с с с с н с с н н н н н н н н н н н н н н н н н н н н	3.323031 0.421141 -0.384801 1.249282 0.061592 1.695920 -1.621436 -2.276934 -2.276934 -2.889394 -2.904764 -1.459304 -3.283778 -2.509885 -2.829439 -4.541490 -4.672645 -4.685176 -4.281362 -4.958682 -5.706630 -1.666510 -3.081506 -4.403466 -4.019437 -2.128865 -1.776699 1.218805 -3.380418 -0.391566 -2.645281 -6.111209	-3.048286 -4.150918 -3.553714 -4.180079 -5.176328 -4.232875 -1.068930 -2.041595 -2.914821 -1.388607 -2.408199 0.470683 0.639671 0.023083 -0.338127 -0.896858 -1.221033 -0.479129 0.372308 -1.607200 1.322600 1.045794 -1.135275 -2.083892 -0.796959 -4.343395 -2.740683 -4.415785 -2.805590 0.771232 0.971020	$\begin{array}{c} 1.046528\\ -0.948637\\ -1.384426\\ -1.659088\\ -0.805816\\ 0.751993\\ -0.915275\\ -2.520898\\ -2.247764\\ -3.145138\\ -3.157343\\ -0.447295\\ 0.659690\\ 2.002883\\ -0.434341\\ -1.358325\\ 0.801669\\ 2.081513\\ 2.220653\\ 0.870262\\ 0.610303\\ -1.347141\\ 2.950765\\ 0.650567\\ 2.211943\\ 0.315841\\ 2.949757\\ 2.180985\\ 4.822501\\ 2.785069\\ -0.529961\\ \end{array}$

ĩ	С	-1.118487	4.143563	-2.547799	С	-3.174764	2.300749	0.610005
	С	-0.294114	4.889684	-1.664181	Н	-2.354725	2.469364	1.307350
ALL I	С	0.486701	4.197189	-0.678947	Н	-2.850498	2.587938	-0.392817
	С	1.252832	4.976764	0.232258	Н	-4.005467	2.954195	0.896520
1. Do 1	С	1.269052	6.352199	0.154417	Н	-4.541339	0.825847	-0.050916
	С	0.524313	7.028777	-0.840271	С	-3.262347	-2.573977	0.833098
	С	-0.242280	6.308186	-1.726847	Н	-2.249598	-2.983503	0.819991
	Ĥ	-0.832344	6 815269	-2 486653	н	-3 454433	-2 161326	1 825321
	н	0.551631	8 113/72	-0.89/110	н	-3 969197	-3 39/226	0.667340
	ц	1 857050	6 023204	0.867632	и Ц	4 511532	1 207303	0.107567
b—4	11	1.83/039	0.923204	0.807032	C ···	-4.511552	-1.207303	-0.197307
TS1	н	1.824590	4.4/4311	1.003939	Cu	0.43301/	-2.0/69/5	0.16//8/
(R)-SN2	Н	-1.689015	4.669849	-3.308833	C	0.2029/0	-3.1436/0	1.83/344
	Ν	-2.749951	-0.196269	0.128506	Н	-0.104187	-4.168240	1.608270
P -1.083316 -0.169012 -0.046866	С	-3.692493	0.858481	0.644481	Н	1.144158	-3.140661	2.389967
O -0.634457 0.864834 1.167191	С	-4.234638	0.505097	2.028029	Н	-0.579629	-2.623768	2.399035
C 0.760743 1.069628 1.182817	С	-3.385452	0.394043	3.139678	С	2.329477	-2.048510	-0.893962
C 1.322480 1.971681 0.294170	С	-3.905345	0.105089	4.400882	С	1.623240	-1.741980	-2.036909
C 2.762803 2.030187 0.229614	Ĉ	-5 281499	-0.073735	4 573553	Č	0.932095	-2 816730	-2 839126
C = 3.536114 = 1.201369 = 1.111767	Č	-6 13/030	0.039/91	3 476007	č	2 132181	-3 318279	-0.254756
C = 4.953766 = 1.185574 = 1.004662	c	-0.134030	0.037471	2 212114	11	2.132101	2 471412	-0.234730
C = 5.505520 = 1.071175 = 0.075260	U U	-3.0104/3	0.5258/1	2.212114	П	2.079091	-5.4/1415	0.073930
C 3.393320 1.9/11/3 0.0/3200	Н	-6.282241	0.414/03	1.360325	C	1.677823	-4.509000	-1.0/4412
C 4.839/14 2.790394 -0.795863	Н	-7.205140	-0.097416	3.598621	С	1.575628	-4.190149	-2.577800
C 3.463045 2.814692 -0.729292	Н	-5.683430	-0.299728	5.557392	Н	2.585866	-4.182710	-3.005226
Н 2.904801 3.427491 -1.427065	Н	-3.235196	0.020624	5.252236	Н	2.407616	-5.312474	-0.907652
Н 5.348828 3.395181 -1.541956	Η	-2.315625	0.531446	3.013361	Н	1.635833	-0.725788	-2.420804
Н 6.678276 1.945946 -0.008078	С	-3.450768	-1.481271	-0.225797	Н	2.938856	-1.316166	-0.368718
H 5 503355 0 495944 1 638289	Č	-3 176819	-1 932933	-1 665379	н	1 014165	-4 975767	-3 095177
C = 2.885010 = 0.360463 = 2.054594	Č	2 072565	3 280015	1 005828	ц	0.726285	4.979707	0.688728
C = 1.512204 = 0.280170 = 2.095646	C	-2.972303	-3.280013	-1.993626	11	0.142706	-4.09/941	-0.088728
C = 1.312304 = 0.289179 = 2.083040	C	-2.824191	-3.6/8901	-3.328464	н	-0.143/96	-2.846222	-2.606130
H 3.4868/8 -0.291133 2.6/9690	С	-2.875981	-2.737033	-4.355062	Н	-2.936/33	-4.033/80	-1.216/62
C 0.444531 2.758904 -0.616527	С	-3.079399	-1.390656	-4.039505	Н	-3.386121	0.052211	-2.477481
C -0.460696 2.103928 -1.440774	С	-3.229997	-0.996797	-2.711497	Н	-2.671989	-4.730153	-3.558595
O -0.613445 0.723811 -1.387448	Η	-2.763291	-3.046522	-5.390416	Н	-3.125619	-0.647023	-4.830697
C -1.217232 2.779721 -2.426392	Н	0.992924	-0.371953	2.771318	Н	0.986622	-2.559635	-3.904259
	Н	-1 857684	2 193161	-3 077446	Br	4 732488	-2.640679	1 712376
Q	C	2 441524	1 802122	2 276248	ц	0 487024	0.015702	2 526691
۰. J	C	-2.441534	1.803132	3.376348	Н	-0.487034	0.915793	3.536684
. X.	C C	-2.441534 -3.549862	1.803132 2.065945	3.376348 2.528050	H C	-0.487034 0.329812	0.915793 3.398377	3.536684 0.644746
xtr	C C C	-2.441534 -3.549862 -3.558565	1.803132 2.065945 1.536223	3.376348 2.528050 1.193742	H C H	-0.487034 0.329812 -0.357778	0.915793 3.398377 3.248635	3.536684 0.644746 -0.188062
xxt	C C C C	-2.441534 -3.549862 -3.558565 -4.649062	1.803132 2.065945 1.536223 1.881630	3.376348 2.528050 1.193742 0.348524	H C H H	-0.487034 0.329812 -0.357778 -0.082796	0.915793 3.398377 3.248635 2.923958	3.536684 0.644746 -0.188062 1.538245
the second	C C C C C C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314	1.803132 2.065945 1.536223 1.881630 2.672199	3.376348 2.528050 1.193742 0.348524 0.805327	H C H H	-0.487034 0.329812 -0.357778 -0.082796 0.394653	0.915793 3.398377 3.248635 2.923958 4.473840	3.536684 0.644746 -0.188062 1.538245 0.837265
A A	C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907	Н С Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195
A A A	C C C C C C C C C C C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497	Н С Н Н Н С	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155
XXX	C C C C C C C C H	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282	H C H H H C H	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270
XXX	C C C C C C C C H H	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228	H C H H H C H	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521
	C C C C C C C C H H H	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256	H C H H H C H H H	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.837521
	C C C C C C C C C H H H H	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 4.66092	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.539261	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 0.676192	Н С Н Н Н С Н Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 2.86777	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744
Int _{re seo}	C C C C C C C C C C H H H H H	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 2.451706	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192	H C H H H C H H H H H	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744
Int _{(R)-SN2}	C C C C C C C C C C C C C C C C C C C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153	H C H H H C H H H H C u	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822	0.915793 3.398377 3.248635 2.923958 4.473840 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 2.254469	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689
P 0.754161 0.234611 0.102005	C C C C C C C H H H H H N C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -6.511057 -6.496814 -4.660082 -2.451796 1.894128	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061	H C H H H C H H H H C u C	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920
P 0.754161 0.234611 -0.103995 0 0.32021 1.015710 1.002917	C C C C C C C H H H H H N C	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309	H C H H H C H H H H C u C H	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277
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P 0.754161 0.234611 -0.103995 O -0.320231 1.016710 -1.092817 C -1.420040 0.229436 -1.466550 C -2.462480 0.032492 -0.574145 C -3.510260 -0.878946 -0.968332 C -3.501473 -1.435834 -2.293378 C -4.541887 -2.320518 -2.687715 C -5.537841 -2.677736 -1.808595	СССССННННН КССССССН	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181	Н С Н Н Н Н С И Н Н Н С С С С С Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486
$\begin{array}{c cccc} & & & & & \\ \hline & & & & \\ \hline & & & & \\ \hline & & & &$	ССССССНННННКССССССНИ	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.88442	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 1.530562	Н С Н Н Н С Н Н Н Н С С С С С Н Ч	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 2.257878	0.915793 3.398377 3.248635 2.923958 4.473840 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290	3.536684 0.644746 -0.188062 1.538245 0.837265 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.7494886 -0.625465 -0.625465
$\begin{array}{c c} \\ \hline \\ P & 0.754161 & 0.234611 & -0.103995 \\ O & -0.320231 & 1.016710 & -1.092817 \\ C & -1.420040 & 0.229436 & -1.466550 \\ C & -2.462480 & 0.032492 & -0.574145 \\ C & -3.510260 & -0.878946 & -0.968332 \\ C & -3.501473 & -1.435834 & -2.293378 \\ C & -4.541887 & -2.320518 & -2.687715 \\ C & -5.537841 & -2.677736 & -1.808595 \\ C & -5.526002 & -2.167049 & -0.489297 \\ C & -4.543196 & -1.291863 & -0.080293 \\ \end{array}$	ССССССНННННКОСССССНН.	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 2.87562	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.66257\end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.38309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 2.814300	Н О Н Н Н Н О Н Н Н Н ^С О Н Н Н О О О О Н Н С	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.64920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.522700
$\begin{array}{c cccc} & & & & & \\ \hline & & & & \\ \hline & & & & \\ \hline & & & &$	ССССССННННН КОСССССННН:	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399	Н С Н Н Н Н С Н Н Н Н С ^U С Н Н Н С С С С С Н Н С С	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789
$\begin{array}{c cccc} & & & & \\ \hline \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline \hline \hline \hline$	ССССССННННН И ОССССССНННН.	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502 1.931592	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356 4.159059	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568	Н С Н Н Н Н С Н Н Н Н С С С Н Н Н С С С С Н Н С С	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 -2.686920 -2.749486 -2.686920 -2.443277 -3.351431 -3.108896 -3.51459 -0.749486 -0.625465 -1.603786 0.523789 1.719167
$\begin{array}{c ccccc} & & & & \\ \hline & & \hline \\ \hline & & \\ \hline \hline & & \\ \hline \hline & & \\ \hline \hline & & \\$	ССССССННННН И ОССССССННННН	$\begin{array}{c} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\end{array}$	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ \end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325	Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С	$\begin{array}{c} -0.487034\\ 0.329812\\ -0.357778\\ -0.082796\\ 0.394653\\ 2.354952\\ 3.893786\\ 3.495500\\ 3.644308\\ 4.984527\\ 3.864300\\ 1.112822\\ 1.964480\\ 2.981305\\ 1.475939\\ 1.946010\\ 0.541729\\ 0.228464\\ 1.674485\\ 1.227878\\ 2.354353\\ 2.433075\\ 1.494815\\ 1.196134 \end{array}$	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000 -5.224283	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446
$\begin{array}{c ccccc} & & & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline &$	ССССССНННННКОСССССНННННО	$\begin{array}{c} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\end{array}$	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091 \end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698	Н С Н Н Н Н С Н Н Н Н С С С Н Н Н С С С Н Н С С Н Н Н С С Н Н Н С С Н Н С С Н Н С С И Н	$\begin{array}{c} -0.487034\\ 0.329812\\ -0.357778\\ -0.082796\\ 0.394653\\ 2.354952\\ 3.893786\\ 3.495500\\ 3.644308\\ 4.984527\\ 3.864300\\ 1.112822\\ 1.964480\\ 2.981305\\ 1.475939\\ 1.946010\\ 0.541729\\ -0.238849\\ 0.228464\\ 1.674485\\ 1.227878\\ 2.354353\\ 2.433075\\ 1.494815\\ 1.196134\\ 3.172023\end{array}$	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475 -4.270000 -5.224283 -5.280728	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019
$\begin{array}{c c} \\ \hline \\ P & 0.754161 & 0.234611 & -0.103995 \\ O & -0.320231 & 1.016710 & -1.092817 \\ C & -1.420040 & 0.229436 & -1.466550 \\ C & -2.462480 & 0.032492 & -0.574145 \\ C & -3.510260 & -0.878946 & -0.968332 \\ C & -3.501473 & -1.435834 & -2.293378 \\ C & -4.541887 & -2.320518 & -2.687715 \\ C & -5.537841 & -2.677736 & -1.808595 \\ C & -5.526002 & -2.167049 & -0.489297 \\ C & -4.543196 & -1.291863 & -0.080393 \\ H & -4.552200 & -0.913204 & 0.934602 \\ H & -6.300723 & -2.467912 & 0.210050 \\ H & -6.326406 & -3.356395 & -2.119711 \\ H & -4.529761 & -2.717164 & -3.699763 \\ \end{array}$	ССССССНННННКСССССССНННННСС	$\begin{array}{c} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\\ 3.565654\end{array}$	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091\\ -0.096889\\ \end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.38309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929	Н О Н Н Н Н О Н Н Н Н ^U О Н Н Н О О О О Н Н О О Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183	0.915793 3.398377 3.248635 2.923958 4.473840 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.917801 -5.918290 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.648920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212
$\begin{array}{c} \\ \hline \\ P & 0.754161 \\ 0.234611 \\ 0.234611 \\ 0.103995 \\ 0.320231 \\ 1.016710 \\ 0.229436 \\ -1.466550 \\ 0.320231 \\ 1.016710 \\ -1.092817 \\ 0.29436 \\ -1.466550 \\ 0.229436 \\ -1.466550 \\ 0.229436 \\ -1.466550 \\ 0.32492 \\ -0.574145 \\ 0.32492 \\ -0.574145 \\ 0.32492 \\ -3.510260 \\ -0.878946 \\ -0.968332 \\ 0.32492 \\ -3.501473 \\ -1.435834 \\ -2.293378 \\ 0.351473 \\ -2.320518 \\ -2.687715 \\ 0.3512841 \\ -2.677736 \\ -1.808595 \\ 0.352002 \\ -2.167049 \\ -0.489297 \\ 0.4541887 \\ -1.291863 \\ -0.80393 \\ H \\ -4.552200 \\ -0.913204 \\ 0.934602 \\ H \\ -6.300723 \\ -2.467912 \\ 0.210050 \\ H \\ -6.326406 \\ -3.356395 \\ -2.119711 \\ H \\ -4.529761 \\ -2.717164 \\ -3.699763 \\ C \\ -2.442106 \\ -1.111759 \\ -3.182840 \\ \end{array}$	ССССССНННННИСССССССНННННССС	$\begin{array}{c} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.359621\\ 3.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\\ 3.565654\\ 4.474707\end{array}$	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648005\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091\\ -0.096889\\ -1.151674\end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312	Н О Н Н Н Н О Н Н Н Н О'О Н Н Н О С О О Н Н С О Н Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.496134 3.172023 -1.206183 0.004360	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.672492 -3.063644 -1.345646 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913
$\begin{array}{c cccc} & & & \\ \hline & & $	ССССССНННННИССССССНННННОССС	$\begin{array}{r} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\\ 3.565654\\ 4.474707\\ 4.764264\end{array}$	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356 4.159059 2.879050 0.946091 -0.096889 -1.151674 -2.024976	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227	Н С Н Н Н Н С Н Н Н Н С С С Н Н Н С С С С Н Н Н С Н Н Н Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.23849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183 0.004360 2.014877	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212
$\begin{array}{c ccccc} & & & & \\ \hline & & & & \\ \hline & & & & \\ \hline & & & &$	ССССССНННННИСССССССНННННССССС	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502 1.931592 0.963276 3.328363 3.565654 4.474707 4.764264 4.149428	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356 4.159059 2.879050 0.946091 -0.096889 -1.151674 -2.024976 -1.859974	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535	Н О Н Н Н Н О Н Н Н Н С О Н Н Н О О О О	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183 0.004360 2.014877 2.998422	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489 -3.59159	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939
$\begin{array}{c c} \\ \hline \\ $	ССССССНННННИСССССССНННННОСССССС	$\begin{array}{c} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\\ 3.565654\\ 4.474707\\ 4.764264\\ 4.149428\\ 3.200827\\ \end{array}$	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356 4.159059 2.879050 0.946091 -0.096889 -1.151674 -2.024976	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535 3.62100	Н С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183 0.004360 2.014877 2.998422 2.0383254	0.915793 3.398377 3.248635 2.923958 4.473840 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489 -3.594559 -3.167464	3.536684 0.644746 -0.188062 1.538245 0.837265 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.646920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939 2.159010
$\begin{array}{c c} \\ \hline \\ $	ССССССНННННИСССССССНННННССССССС	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502 1.931592 0.963276 3.328363 3.565654 4.474707 4.764264 4.149428 3.240982 2.956042	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091\\ -0.096889\\ -1.151674\\ -2.024976\\ -1.859974\\ -0.812241\\ 0.872697\end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.38309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535 3.662109 2.611012	Н О Н Н Н Н О Н Н Н Н С ^и О Н Н Н О О О О Н Н О О Н Н Н Н Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183 0.004360 2.014877 2.998422 -0.383854	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.991702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489 -3.594559 -3.167464 -3.59242	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.648920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939 2.159019
$\begin{array}{c} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	ССССССННННН И ОССССССННННН И ОССССС:	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502 1.931592 0.963276 3.328363 3.565654 4.474707 4.764264 4.149428 3.240982 2.956042 2.956042	1.803132 2.065945 1.536223 1.881630 2.672199 3.159696 2.863436 3.247249 3.775982 2.928775 1.529261 2.188927 1.405108 2.902157 3.648605 3.533647 4.254750 5.104455 5.228902 4.502950 4.611356 5.888433 5.666356 4.159059 2.879050 0.946091 -0.096889 -1.151674 -2.024976 -1.859974 -0.812241 0.057688	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535 3.662109 2.611013	Н О Н Н Н Н О Н Н Н Н И О О Н Н Н О С О О Н Н Н С О Н Н Н Н Н Н	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.496134 3.172023 -1.206183 0.004360 2.014877 2.998422 -0.383854 4.985521 2.25551	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489 -3.594559 -3.167464 -1.289342 -9.672672	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939 2.159019 0.239195
$\begin{array}{c c} \\ \hline \\ $	СССССССННННН И ОСССССОННННН ОСССССН:	-2.441534 -3.549862 -3.558565 -4.649062 -5.681314 -5.687245 -4.638467 -4.619173 -6.511057 -6.496814 -4.660082 -2.451796 1.894128 1.745643 2.351262 1.812762 2.359621 3.449936 3.989032 3.441703 3.863928 4.834064 3.872502 1.931592 0.963276 3.328363 3.565654 4.474707 4.764264 4.149428 3.240982 2.956042 4.387526	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.53647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091\\ -0.096889\\ -1.151674\\ -2.024976\\ -1.859974\\ -0.812241\\ 0.057688\\ -2.527361\\ 0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -2.527361\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.97688\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.9768\\ -0.$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 -2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535 3.662109 2.611013 4.305073	Н О Н Н Н Н О Н Н Н Н И О О Н Н Н О О О О	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.23849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -0.206183 -1.206183 0.004360 2.014877 2.998422 -0.383854 4.985521 2.255910 	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475 -4.270000 -5.224283 -5.280728 -3.009438 -4.115765 -3.713489 -3.594559 -3.167464 -1.289342 0.872878	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -1.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939 2.159019 0.239195 2.7677116
$\begin{array}{c cccc} & & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline & & $	ССССССНННННИСССССССНННННССССССНН	$\begin{array}{r} -2.441534\\ -3.549862\\ -3.558565\\ -4.649062\\ -5.681314\\ -5.687245\\ -4.638467\\ -4.619173\\ -6.511057\\ -6.496814\\ -4.660082\\ -2.451796\\ 1.894128\\ 1.745643\\ 2.351262\\ 1.812762\\ 2.359621\\ 3.449936\\ 3.989032\\ 3.441703\\ 3.863928\\ 4.834064\\ 3.872502\\ 1.931592\\ 0.963276\\ 3.328363\\ 3.565654\\ 4.474707\\ 4.764264\\ 4.149428\\ 3.240982\\ 2.956042\\ 4.387526\\ -0.576515\end{array}$	$\begin{array}{c} 1.803132\\ 2.065945\\ 1.536223\\ 1.881630\\ 2.672199\\ 3.159696\\ 2.863436\\ 3.247249\\ 3.775982\\ 2.928775\\ 1.529261\\ 2.188927\\ 1.405108\\ 2.902157\\ 3.648605\\ 3.533647\\ 4.254750\\ 5.104455\\ 5.228902\\ 4.502950\\ 4.611356\\ 5.888433\\ 5.666356\\ 4.159059\\ 2.879050\\ 0.946091\\ -0.096889\\ -1.151674\\ -2.024976\\ -1.859974\\ -0.812241\\ 0.057688\\ -2.527361\\ -0.064199\end{array}$	3.376348 2.528050 1.193742 0.348524 0.805327 2.132907 2.972497 3.989282 2.480228 0.135256 -0.676192 4.392153 0.185061 0.338309 -0.846605 -2.137493 -3.198362 2.986433 -1.706597 -0.645009 0.352181 -1.530563 -3.814399 -4.192568 -2.310325 0.256698 1.353929 1.186312 2.240227 3.481535 3.662109 2.611013 4.305073 -3.429427	Н О Н Н Н Н О Н Н Н Н И О О И Н Н О О О О	-0.487034 0.329812 -0.357778 -0.082796 0.394653 2.354952 3.893786 3.495500 3.644308 4.984527 3.864300 1.112822 1.964480 2.981305 1.475939 1.946010 0.541729 -0.238849 0.228464 1.674485 1.227878 2.354353 2.433075 1.494815 1.196134 3.172023 -1.206183 0.004360 2.014877 2.998422 -0.383854 4.985521 2.255910 5.485018	0.915793 3.398377 3.248635 2.923958 4.473840 3.139796 0.582139 -0.366979 1.368341 0.499281 1.846787 -1.988448 -2.354108 -2.672492 -3.063644 -1.345646 -3.966592 -3.470166 -3.562545 -4.917801 -5.918290 -4.91702 -4.515475 -4.270000 -5.224283 -5.280728 -3.09438 -4.115765 -3.713489 -3.594559 -3.167464 -1.289342 0.872878 -2.824291 -2.672492 -2.672492 -3.594559 -3.167464 -1.289342 0.872878 -2.824291 -2.672492 -2.672492 -2.672492 -2.672492 -2.672492 -3.594559 -3.167464 -1.289342 0.872878 -2.824291 -2.672492 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.824291 -2.672492 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.824291 -2.672492 -2.672492 -2.824291 -2.672492 -2.824291 -2.672492 -2.824291 -2.672492 -2.824291 -2.672492 -2.824291 -2.824291 -2.672492 -2.824291 -2.824291 -2.672492 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.824291 -2.82	3.536684 0.644746 -0.188062 1.538245 0.837265 1.219195 -1.122155 -1.493270 -1.837521 -1.082485 0.574744 -0.916689 -2.686920 -2.443277 -3.351431 -3.108896 -0.051462 0.068492 1.351459 -0.749486 -0.625465 -1.603786 0.523789 1.719167 2.186446 0.781019 -0.120212 -1.982913 2.508635 0.326939 2.159019 0.239195 2.767716 2.090277

▲ Î	С	-2.322243	1.789592	3.417992	Н	-0.430032	0.776501	3.563267
· · · · · · · · · · · · · · · · · · ·	С	-3.386866	2.179353	2.562669	С	0.698266	3.267229	0.927779
respective de Provincia de Prov	С	-3.390691	1.738378	1.196812	Н	-0.035104	3.224334	0.121538
1 March March	С	-4.429754	2.213156	0.349388	Н	0.296323	2.753765	1.803814
	С	-5.419731	3.041986	0.831793	Н	0.841008	4.319064	1.193787
	С	-5.433750	3.440201	2.188575	Н	2.718832	2.815567	1.388401
	С	-4.432626	3.018116	3.032567	С	3.966497	0.434841	-1.265636
I I I	Ĥ	-4 417197	3 332873	4 072844	Ĥ	3 452177	-0 404154	-1 743886
	н	-6 224461	4 087748	2 555370	н	3 781646	1 334195	-1 855715
$I \neq 2$	ц	6 10/606	3 308584	0.150374	ц	5 042102	0.234031	1 200777
	11	4 422508	1 022054	0.137374	11	4 100024	1 475772	-1.270777
1 S2 _{(R)-SN2}	п	-4.435308	1.932034	-0.097200	п	4.100024	1.4/3//2	0.374343
	H	-2.330324	2.10/354	4.45/02/	Cu	1.058555	-2.052922	-0.836/69
P 0.844400 0.182282 -0.116735	N	2.089692	1.224546	0.222930	U U	2.38/419	-3.016/84	-2.045060
O -0.147068 1.100869 -1.074995	C	2.061941	2.707299	0.516297	Н	3.241/10	-2./35294	-1.423014
C -1.299298 0.428935 -1.504004	С	2.675704	3.524350	-0.616780	Н	2.475379	-4.052679	-2.355074
C -2.366349 0.266263 -0.634927	С	2.085584	3.573952	-1.889100	Н	2.266528	-2.365139	-2.915606
C -3.472956 -0.542035 -1.089956	С	2.641009	4.363874	-2.895113	С	0.442146	-4.045664	-1.135129
C -3.485229 -1.028278 -2.442679	С	3.790828	5.119653	-2.645373	С	-0.772466	-3.347989	-0.688013
C -4 581099 -1 813260 -2 894882	С	4.381903	5.080029	-1.383098	С	-1.123835	-3.288916	0.625840
C = 5.612520 = 2.144067 = 2.046823	С	3.826332	4.284819	-0.376962	С	1.072755	-4.976646	-0.119307
C = 5.582722 = 1.706008 = 0.702108	Н	4.290038	4.264358	0.607380	Н	0.475003	-5.902359	-0.125819
C = 4.546165 = 0.925513 = 0.236881	Н	5.273865	5.665183	-1.178042	Н	2.085549	-5.261336	-0.418534
H = 4.546165 - 0.525515 - 0.256881	Н	4.219618	5.735852	-3.430399	С	1.071194	-4.365416	1.289777
11 -4.540250 -0.590059 0.795559	Н	2 173497	4 395320	-3 875546	Ċ	-0 337794	-3 932142	1 727984
H = -0.38/35/ = -1.985090 = -0.028180	н	1 1916/18	2 990986	-2 090730	н	-0.920254	_1 799039	2 080935
H -0.442925 -2.740749 -2.402215	C	3 /86310	0.660862	0.174859	н	1 485563	-5.078853	2.000933
H -4.582884 -2.155850 -3.926521	c	2 685050	0.523506	1 1 2 8 0 6 4	и П	1.405505	2 008242	1 420227
C -2.390836 -0.738942 -3.302242	C	5.085050	-0.323300	1.128004	п	-1.424301	-2.908242	-1.43923/
C -1.300183 -0.045826 -2.834801	C	4.330029	-1.3/9/43	0.820328	п	0.380030	-4.411037	-2.134691
Н -2.420535 -1.086935 -4.331319	C	4.811343	-2.595938	1./46429	н	-0.284845	-3.251454	2.58/066
C -2.333031 0.875872 0.725038	С	4.203852	-2.573239	3.001897	Н	1.741722	-3.494222	1.306905
C -1.269201 0.636907 1.583675	С	3.338933	-1.524000	3.324710	Н	-2.061809	-2.804689	0.888963
O -0.161122 -0.107441 1.181367	С	3.085935	-0.511707	2.399546	Н	5.064062	-1.608320	-0.137853
C -1.269606 1.054110 2.934141	Н	4.411433	-3.355714	3.726132	Н	2.419440	0.301802	2.668831
	Н	-0.447459	0.176471	-3.468874	Н	5.498545	-3.396476	1.486555
					Н	2.871265	-1.485520	4.304784
3.1	С	-4.301555	1.536444	2.183960	С	-0.382532	3.591712	0.638114
	C C C C C C H	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439	C H H H C H	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037
	C C C C C C H H	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067	C H H H C H H	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100
A CHA	C C C C C C H H H	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771	C H H H C H H H	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440
	C C C C C C H H H H	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452	С Н Н Н С Н Н Н Н	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179
C2 _{(R)-SN2}	C C C C C C C H H H H H	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911	C H H C H H H H Cu	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535
C2 _{(R)-SN2}	C C C C C C C H H H H H N	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480	C H H H C H H H H C u C	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891
Р 0.547790 0.556721 0.051576	C C C C C C C C H H H H H H N C	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435	C H H H C H H H H C u C H	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.463100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108
P 0.547790 0.556721 0.051576 O -0.580055 1.003427 -1.071063	C C C C C C H H H H H N C C	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220	C H H H C H H H H C U C H H H H H C H H H H	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 0.520179 -0.288535 -1.683891 -0.836108 -1.926569
P 0.547790 0.556721 0.051576 O -0.580055 1.003427 -1.071063 C -1.423117 -0.063353 -1.425175	С С С С С С Н Н Н Н Н N С С С	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032	С Н Н Н Н С Н Н Н Н С С Н Н Н Н Н Н С И Н Н Н И С И Н Н И С И И И И	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326
P 0.547790 0.556721 0.051576 O -0.580055 1.003427 -1.071063 C -1.423117 -0.063353 -1.425175 C -2.453173 -0.434828 -0.576343	С С С С С С Н Н Н Н Н N С С С С С	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808	С Н Н Н Н С Н Н Н Н С С Н Н Н С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863
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P 0.547790 0.556721 0.051576 O -0.580055 1.003427 -1.071063 C -1.423117 -0.063353 -1.425175 C -2.453173 -0.434828 -0.576343 C -3.198978 -1.622140 -0.920740 C -2.932930 -2.287362 -2.166670	ССССННННКСССССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.055872 \\ \hline \\ P & 0.547790 \\ 0.556721 \\ 0.058055 \\ 1.003427 \\ -1.071063 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ \hline \end{array}$	ССССННННИСССССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.676282	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177
P 0.547790 0.556721 0.051576 O -0.580055 1.003427 -1.071063 C -1.423117 -0.063353 -1.425175 C -2.453173 -0.434828 -0.576343 C -3.198978 -1.622140 -0.920740 C -2.932930 -2.287362 -2.166670 C -3.676345 -3.448387 -2.512709 C -4.622219 -3.963179 -1.656572	СССССННННИССССССН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709	С Н Н Н Н С Н Н Н Н С С Н Н Н Н С С С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5 947166	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ C & -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ \end{array}$	СССССН Н Н Н Н N ССССССН Н	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452	С Н Н Н Н С Н Н Н Н С С С Н Н Н Н С С С С С Н Н	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ C & -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.62219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.37296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.051787 \\ \end{array}$	СССССНННННКССССССННН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028	С Н Н Н Н С Н Н Н Н С С С С С Н Н С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.27123	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 0.0091613 1.213926
$\begin{array}{c} \\ \hline \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051777 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0$	СССССНННННКССССССНННН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 4.250600	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.29841	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926
$\begin{array}{c} \\ \hline \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0 & -0.580055 \\ 1.003427 \\ -1.071063 \\ C & -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.37296 \\ -0.051787 \\ H & -4.359380 \\ -1.735808 \\ 0.908608 \\ H & -5.586332 \\ -3.759001 \\ 0.972483 \\ \end{array}$	СССССНННННКССССССНННН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146	СННННСННННССНННСССННССИ	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965700	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.0558055 \\ 1.003427 \\ -1.071063 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.57808 \\ -0.57808 \\ -0.579091 \\ -0.57808 \\ -0.579091 \\ -0.274483 \\ H & -5.586332 \\ -3.759091 \\ -2.27483 \\ -1.735808 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -1.92590 \\ -$	СССССНННННИССССССНННННС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н И	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.0556721 \\ 0.0556721 \\ 0.0556721 \\ 0.055702 \\ 0.0556721 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.103427 \\ -1.071063 \\ 0.103427 \\ -1.071063 \\ 0.103427 \\ -1.071063 \\ 0.103427 \\ -1.071063 \\ 0.103427 \\ -1.071063 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051576 \\ 0.051577 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 \\ 0.051787 $	СССССННННН ИСССССССНННННСС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710632	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н Н Ч	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -3.274280	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 2.117706
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.05353 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ 0.2.453173 \\ -0.434828 \\ -0.576343 \\ 0.576343 \\ 0.576343 \\ 0.52140 \\ -0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0$	СССССНННННОССССССНННННССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.4877711 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С О Н Н С С Н Н Н И	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.095878	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -3.9274380 -3.274380 -3.274380 -3.274380	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0555 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ 0.2.453173 \\ -0.434828 \\ -0.576343 \\ 0.576343 \\ 0.3.198978 \\ -1.622140 \\ -0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.920740 \\ 0.9207$	СССССНННННКОССССССНННННСССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.990174 4.926618	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 0.712427	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.4877711 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.085878 2.988797	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 2.65720	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 -2.06022
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0.0555 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.0580055 \\ 1.003427 \\ -1.071063 \\ 0.051576 \\ 0.05353 \\ -1.425175 \\ 0.2453173 \\ -0.434828 \\ -0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ 0.576343 \\ -2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.2.932930 \\ -2.287362 \\ -2.166670 \\ 0.572179 \\ 0.56572 \\ -3.676345 \\ -3.448387 \\ -5.182570 \\ -3.37296 \\ -0.051787 \\ H \\ -4.359380 \\ -1.735808 \\ 0.908608 \\ H \\ -5.586332 \\ -3.759091 \\ 0.274483 \\ H \\ -5.182570 \\ -4.852402 \\ -1.929529 \\ H \\ -3.476188 \\ -3.927979 \\ -3.467510 \\ 0.21422 \\ -1.929529 \\ H \\ -3.476188 \\ -3.927979 \\ -3.467510 \\ 0.21422 \\ -2.651425 \\ H \\ -1.742302 \\ -2.93096 \\ -2.070202 \\ \end{array}$	СССССНННННКССССССНННННССССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 -0.172427 -0.969626	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.085878 2.988797 1.037861	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 -3.665720 -3.265720	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 2.086922 1.254202
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0 & -0.580055 \\ 1.003427 \\ -1.071063 \\ C & -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.37296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.051787 \\ H & -4.359380 \\ -1.735808 \\ 0.908608 \\ H & -5.586332 \\ -3.759091 \\ 0.274483 \\ H \\ -5.182570 \\ -4.852402 \\ -1.92529 \\ H \\ -3.476188 \\ -3.927979 \\ -3.467510 \\ C \\ -1.916125 \\ -1.789344 \\ -3.025629 \\ C \\ -1.150598 \\ -0.710742 \\ -2.651425 \\ H \\ -1.743203 \\ -2.280956 \\ -3.979392 \\ C \\ -2.736217 \\ 0.250246 \\ 0.452920 \\ \end{array}$	СССССНННННКССССССНННННССССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618 4.313237	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 -0.172427 -0.969626 -0.898727	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691 3.516216	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.085878 2.988797 1.037861 3.349679	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 -3.665720 -3.320553	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.35775 2.060797 -2.117796 -2.212730 2.086922 1.354800
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.051576 \\ 0 & -0.580055 \\ 1.003427 \\ -1.071063 \\ C & -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.57808 \\ 0.051787 \\ H \\ -4.359380 \\ -1.735808 \\ 0.908608 \\ H \\ -5.586332 \\ -3.759091 \\ 0.274483 \\ H \\ -5.182570 \\ -4.852402 \\ -1.929529 \\ H \\ -3.476188 \\ -3.927979 \\ -3.467510 \\ C \\ -1.916125 \\ -1.789344 \\ -3.025629 \\ C \\ -1.150598 \\ -0.710742 \\ -2.651425 \\ H \\ -1.743203 \\ -2.280956 \\ -3.979392 \\ C \\ -2.736217 \\ 0.359246 \\ 0.652380 \\ \end{array}$	СССССНННННКССССССНННННКСССССС	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618 4.313237 3.242837 2.90176	$\begin{array}{c} 1.536444\\ 0.898320\\ 0.864256\\ 1.396149\\ 1.987588\\ 2.057710\\ 2.527614\\ 2.395776\\ 1.366053\\ 0.427911\\ 2.120319\\ 1.901418\\ 3.354763\\ 4.140719\\ 3.878687\\ 4.639936\\ 5.676282\\ 5.946486\\ 5.180418\\ 5.402407\\ 6.751425\\ 6.269354\\ 4.429284\\ 3.077463\\ 1.668978\\ 0.710628\\ -0.172427\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.898727\\ -0.969626\\ -0.89872\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.96926\\ -0.89872\\ -0.9692\\ -0.9982\\ -0.9982\\ -0.9982\\ -0.9982\\ -0.9982\\ -0.9982\\ -0.998$	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691 3.516216 3.696984 2.641927	С Н Н Н Н С Н Н Н Н И С С Н Н Н С С С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.085878 2.988797 1.037861 3.349679 -0.219646	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 -3.665720 -3.320553 -3.465162	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 2.086922 1.354800 -0.097353
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.0558055 \\ 1.003427 \\ -1.071063 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.576343 \\ -5.586332 \\ -3.759091 \\ 0.274483 \\ H & -5.182570 \\ -4.852402 \\ -1.735808 \\ -1.735808 \\ -0.92529 \\ H & -3.476188 \\ -3.927979 \\ -3.467510 \\ C & -1.916125 \\ -1.789344 \\ -3.025629 \\ C \\ -1.150598 \\ -0.710742 \\ -2.651425 \\ H \\ -1.743203 \\ -2.280956 \\ -3.979392 \\ C \\ -2.736217 \\ 0.359246 \\ 0.652380 \\ C \\ -1.733416 \\ 0.618223 \\ 1.575191 \\ \end{array}$	СССССННННН И ОСССССИННННОССССС:	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -5.770172 -7.581169 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618 4.313237 3.242837 2.801769	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 0.172427 -0.969626 -0.898727 -0.018535 0.777973	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.487771 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691 3.516216 3.696984 2.641327	С Н Н Н Н С Н Н Н Н И С С Н Н Н С С С С	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.085878 2.988797 1.037861 3.349679 -0.219646 5.011484	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 -3.3655720 -3.320553 -3.465162 -0.227262	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 2.086922 1.354800 -0.097353 0.261447
$\begin{array}{c} \\ P & 0.547790 \\ 0.556721 \\ 0.0558055 \\ 1.003427 \\ -1.071063 \\ -1.423117 \\ -0.063353 \\ -1.423117 \\ -0.063353 \\ -1.425175 \\ C & -2.453173 \\ -0.434828 \\ -0.576343 \\ C & -3.198978 \\ -1.622140 \\ -0.920740 \\ C & -2.932930 \\ -2.287362 \\ -2.166670 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -3.676345 \\ -3.448387 \\ -2.512709 \\ C & -4.622219 \\ -3.963179 \\ -1.656572 \\ C & -4.855702 \\ -3.337296 \\ -0.409602 \\ C & -4.166961 \\ -2.198453 \\ -0.51787 \\ H \\ -4.359380 \\ -1.735808 \\ 0.908608 \\ H \\ -5.586332 \\ -3.759091 \\ 0.274483 \\ H \\ -5.182570 \\ -4.852402 \\ -1.929529 \\ H \\ -3.476188 \\ -3.927979 \\ -3.467510 \\ C \\ -1.916125 \\ -1.789344 \\ -3.025629 \\ C \\ -1.150598 \\ -0.710742 \\ -2.651425 \\ H \\ -1.743203 \\ -2.280956 \\ -3.979392 \\ C \\ -2.736217 \\ 0.359246 \\ 0.652380 \\ C \\ -1.733416 \\ 0.618223 \\ 1.575191 \\ 0 \\ -0.415753 \\ 0.207706 \\ 1.356353 \\ 0 \\ -1.01005 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ -0.0105 \\ $	СССССНННННИСССССССНННННССССССН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.41766 2.337859 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618 4.313237 3.242837 2.801769 4.664786	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 0.172427 -0.969626 -0.898727 -0.018535 0.777973 -1.511012	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.4877711 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691 3.516216 3.696984 2.641327 -4.341517	СННННСННННССННННССССННССНННННННН	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.525639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.241722 1.037861 3.349679 -0.219646 5.011484 1.973982	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.249841 -5.254362 -4.249841 -5.254362 -4.249841 -3.274380 -3.274380 -3.320553 -3.465162 -0.227262 1.462071	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 2.086922 1.354800 -0.097353 0.261447 2.800946
$\begin{array}{c} \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	СССССННННИОССССССНННННССССССНН	-4.301555 -4.047671 -5.103608 -6.341527 -6.598526 -5.594291 -7.781169 -7.126940 -4.926474 -3.453400 1.490720 1.097983 1.547514 1.017277 1.411766 2.387542 2.867143 2.473686 2.885453 3.584691 2.640944 0.991813 0.295097 2.979879 3.412100 4.490174 4.936618 4.313237 3.242837 2.801769 4.664786 -0.362135	1.536444 0.898320 0.864256 1.396149 1.987588 2.057710 2.527614 2.395776 1.366053 0.427911 2.120319 1.901418 3.354763 4.140719 3.878687 4.639936 5.676282 5.946486 5.180418 5.402407 6.751425 6.269354 4.429284 3.077463 1.668978 0.710628 0.172427 -0.969626 -0.898727 -0.018535 0.777973 -1.511012 -0.317686	2.183960 0.923704 -0.028401 0.261957 1.520530 2.458215 3.422439 1.737067 -0.4877711 -1.004452 4.090911 0.240480 0.329435 -0.898220 -2.171032 -3.270808 -3.115992 -1.854615 -0.753851 0.228709 -1.723452 -3.974028 -4.250600 -2.300146 0.261064 1.376670 1.211026 2.270691 3.516216 3.696984 2.641327 4.341517 -3.286070	СННННСННННССНННССССННССННННННННН	-0.382532 -1.038017 -0.682883 -0.532156 1.665982 3.52639 3.241176 3.134127 4.617943 3.386017 1.367108 3.999256 4.126252 4.983985 3.661595 3.009528 1.589167 0.849790 3.431918 3.024166 4.522603 2.931722 1.399014 0.965709 3.281722 1.399014 0.965709 3.281722 1.037861 3.349679 -0.219646 5.011484 1.973982 5.783271	3.591712 3.247649 3.112558 4.669526 3.735127 1.330029 0.318384 2.041355 1.394378 2.652977 -1.535692 -2.973746 -2.289139 -3.387057 -2.390271 -4.104386 -3.590704 -3.682601 -4.932415 -5.947166 -5.036208 -4.327123 -4.249841 -5.254362 -4.926661 -3.274380 -4.776897 -3.362553 -3.465162 -0.227262 1.462071 -1.634004	0.638114 -0.163957 1.572932 0.751623 1.187840 -1.133433 -1.448037 -1.863100 -1.153440 0.520179 -0.288535 -1.683891 -0.836108 -1.926569 -2.549326 -1.342863 -1.201219 -0.054046 -0.106177 -0.202860 -0.091613 1.213926 1.231124 1.357775 2.060797 -2.117796 -2.212730 2.086922 1.354800 -0.097353 0.261447 2.800946 2.120655

## 2.1.2. Alkylation of (*S*)-1



**Figure S2.** Energy profiles corresponding to the alkylation of (*S*)-1 by MeCuL1 in both *anti*-S_N2 and *anti*-S_N2' pathways.

Table S5.	Energy	values of al	l stationary	points	relative t	to the	anti-S _N 2	2 pathwa	y in gas ph	ase

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
C1 _{(S)-SN2}	-4977.208413	-4976.466582	-4976.444475	-4976.510908	0.0
TS1 _{(S)-SN2}	-4977.175017	-4976.433692	-4976.411940	-4976.477124	21.2
Int _{(S)-SN2}	-2405.586869	-2404.844357	-2404.823780	-2404.885295	0.0
TS2 _{(S)-SN2}	-2405.585323	-2404.842676	-2404.822418	-2404.883471	1.1
C2 _{(S)-SN2}	-2405.655953	-2404.909699	-2404.889378	-2404.950933	-41.2

Table S6. Energy values of all stationary points relative to the anti-S_N2' pathway in gas phase

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
C1 _{(S)-SN2p}	-4977.208941	-4976.467091	-4976.445511	-4976.510417	0.3
TS1 _{(S)-SN2p}	-4977.166776	-4976.427243	-4976.405179	-4976.471653	24.6
Int _{(S)-SN2p}	-2405.582867	-2404.840654	-2404.819892	-2404.882433	1.8
TS2 _{(S)-SN2p}	-2405.581948	-2404.839415	-2404.819081	-2404.880391	3.1
C2 _{(S)-SN2p}	-2405.652006	-2404.906042	-2404.885538	-2404.948398	-39.6

Table S7. Energy values of all stationary points relative to the anti-S_N2 pathway in dichloromethane (CPCM)

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	ΔG (kcal/mol)
C1 _{(S)-SN2}	-4978.048925	-4977.307094	-4977.284987	-4977.351420	0.0
TS1 _{(S)-SN2}	-4978.039823	-4977.298498	-4977.276746	-4977.341930	6.0
Int _{(S)-SN2}	-2406.468103	-2405.725591	-2405.705014	-2405.766529	0.0
TS2 _{(S)-SN2}	-2406.465726	-2405.723079	-2405.702821	-2405.763874	1.7
C2 _{(S)-SN2}	-2406.536391	-2405.790137	-2405.769816	-2405.831371	-40.7

Coordinate	E (au)	E+ZPE (au)	H (au)	G (au)	∆G (kcal/mol)
C1 _{(S)-SN2p}	-4978.049384	-4977.307534	-4977.285954	-4977.350860	0.3
TS1 _{(S)-SN2p}	-4978.035214	-4977.295681	-4977.273617	-4977.340091	7.1
Int _{(S)-SN2p}	-2406.466158	-2405.723945	-2405.703183	-2405.765724	0.5
TS2 _{(S)-SN2p}	-2406.463340	-2405.720807	-2405.700473	-2405.761783	3.0
C2 _{(S)-SN2p}	-2406.533610	-2405.787646	-2405.767142	-2405.830002	-39.8

Table S8. Energy values of all stationary points relative to the *anti*-S_N2' pathway in dichloromethane (CPCM)

Cartesian coordinates of all stationary points:

Int_{(S)-SN2}, TS2_{(S)-SN2} and C2_{(S)-SN2} are respectively identical to Int_{(R)-SN2p}, TS2_{(R)-SN2p} and C2_{(R)-SN2p}.

Int_{(S)-SN2p}, TS2_{(S)-SN2p} and C2_{(S)-SN2p} are respectively identical to Int_{(R)-SN2}, TS2_{(R)-SN2} and C2_{(R)-SN2}.

			1	С	-3.755752	-0.580613	3.224056	Н	4.746079	2.645183	2.447748
			R	С	-4.557045	-1.311942	2.306923	Н	3.334194	3.257531	0.529434
	a		I Y	С	-4.011136	-1.669622	1.028744	Н	-0.371879	-0.430689	-3.245504
	9		35	С	-4.867184	-2.334572	0.106370	Н	-1.880412	0.425979	3.542212
			9 B	С	-6.165468	-2.655522	0.438848	С	-3.175461	2.415695	0.444984
0	- 1 PN		<u>_</u>	С	-6.685159	-2.335846	1.714731	Н	-3.339023	1.687213	-0.349099
	7-42			С	-5.893447	-1.673886	2.624854	Н	-3.118016	1.890092	1.400685
0	<_ <i>2</i>		$\sum I$	Н	-6.284069	-1.403037	3.603013	Н	-4.042868	3.083420	0.478410
		- L		Н	-7.708185	-2.600929	1.966558	Н	-1.891243	3.988449	1.041968
		9	$\sim r$	Н	-6.798009	-3.154442	-0.290381	С	1.282085	3.806487	-0.869975
		~4	1-2	Н	-4.491534	-2.578362	-0.880520	Н	1.800007	2.927989	-1.269042
	, i	(S)-SN2	0 0	Н	-4.163345	-0.334471	4.201412	Н	0.561384	4.142499	-1.617592
		0.04/00.5		Ν	-0.616688	2.563188	0.255535	Н	2.014061	4.608397	-0.721465
P	-0.208286	0.946205	0.028197	С	-1.932592	3.280285	0.203370	Н	0.088144	4.430109	0.775899
0	-1.401397	0.499201	-1.060270	С	-2.098301	4.115366	-1.066594	Cu	1.950740	0.315340	-0.791501
C	-1.398959	-0.852933	-1.398402	C	-2.090678	3.527336	-2.340422	С	2.589046	0.574618	-2.654795
C	-1.986057	-1.774552	-0.544335	С	-2.287067	4.306238	-3.480335	Н	3.570176	1.072279	-2.681150
C	-1.876548	-3.170740	-0.890529	Ċ	-2,498880	5.683771	-3.368116	Н	2,705739	-0.395151	-3.163427
С	-1.284663	-3.541198	-2.145453	Č	-2.512369	6.277050	-2.106231	Н	1.902037	1.178283	-3.264731
С	-1.187549	-4.915603	-2.493900	Č	-2.311792	5.495024	-0.965451	C	3.665592	-0.630588	0.453519
С	-1.620177	-5.898564	-1.634085	H	-2.323294	5.965107	0.016229	Ċ	2.574542	-0.958193	1 198488
C	-2.162119	-5.540335	-0.377579	Н	-2.673697	7.347235	-2.006149	Ĥ	2.207751	-0.254154	1.941191
С	-2.287937	-4.216375	-0.016907	Н	-2.649576	6.287955	-4.258683	С	1.911218	-2.312745	1.124584
Н	-2.696393	-3.963450	0.954151	Н	-2.273955	3 836778	-4 460563	Č	2.368762	-3 107549	-0 107815
Н	-2.478356	-6.316963	0.313527	Н	-1.920014	2.459445	-2.434888	č	4.371175	-1.615092	-0.439478
Н	-1.534195	-6.945948	-1.909651	C	0.553943	3,494244	0.444425	Ĥ	4.339126	-1.302326	-1.482125
Н	-0.747904	-5.175390	-3.453936	Ċ	1.465543	3.050135	1.593574	С	3.899559	-3.057377	-0.244557
С	-0.774597	-2.531460	-3.004599	Č	2.861105	3 014507	1 474526	Ĥ	4 148654	0 331686	0 597619
С	-0.802489	-1.211497	-2.628432	č	3 665857	2.667123	2 565060	Н	2.037506	-4 149609	-0.030649
Н	-0.331259	-2.820618	-3.953897	Č	3 088742	2 352052	3 794340	н	1 898394	-2 692602	-1.008620
С	-2.651569	-1.311646	0.706614	č	1 697280	2 389718	3 928389	Н	4 247977	-3 676605	-1 077639
С	-1.968936	-0.493861	1.599747	č	0.898921	2,736327	2.840461	н	4 351915	-3 461388	0.669012
0	-0.699874	-0.023630	1.330797	й	-0.181906	2 757379	2 951962	н	0.822723	-2 189948	1 127568
С	-2.499115	-0.160046	2.869900	н	1 235104	2 152080	4 883083	н	2 155189	-2.872161	2.042060
				Н	3.714137	2.082339	4.640875	Br	6.354192	-1.510450	-0.041097

ୁ	C	-3.325477	1.010530	3.328262	Н	4.804014	-0.100021	2.819794
	č	-4 464327	0 701577	2 536571	н	4 069421	0 857046	0 733660
	C	-4 285204	0.081901	1 253827	н	-0.948245	-0 587323	-3 370457
1 a a 🍕	C	-5.442700	-0 140774	0.456400	н	-0.940243 -1.170842	1 029052	3 121723
Soft and the second sec	C C	6 608075	0 10/678	0.012383	C	1 017541	3 20/233	0.102618
ST 490- 1	C	6 972921	0.194078	0.912383	с ц	2 255702	2 760027	0.102018
Share the start		5 775360	1.019357	2.193427	и П	2.333792	2.709027	1 010724
1		-3.//3300	1.016557	2.965236	п	-2.146/99	2.747901	1.019/34
~	H H	-5.8916/5	1.4//058	3.962283	H	-2.38/486	4.281264	0.1/0153
	н н	-/.8/0668	1.021450	2.543160	Н	-0.102553	4.120127	0.808037
	Н	-7.563879	0.021624	0.277861	C	2.823457	2.434635	-0.930843
	Ъ Н	-5.328599	-0.569038	-0.532664	Н	2.921157	1.382949	-1.217357
(S)-5N2	Н	-3.471134	1.461091	4.306727	Н	2.414537	2.980559	-1.784673
D 0 120000 0 (75072 0 1	72570 N	0.467931	2.299954	0.002270	Н	3.828255	2.815972	-0.721661
P = 0.129909 = 0.675972 = 0.11	72570 C	-0.408655	3.518692	-0.057151	Н	1.893709	3.715562	0.473040
0 -1.19/563 0.751/54 -1.1	/834/ C	-0.116337	4.347974	-1.306265	Cu	1.735874	-0.924793	-0.990602
C -1.843025 -0.462646 -1.4	¹⁵⁰⁴⁹ C	-0.278856	3.810378	-2.591661	С	2.190906	-0.850889	-2.927433
C = -2.697562 = -0.992374 = -0.43	59085 C	-0.047238	4.594048	-3.721415	Н	3.267952	-0.849174	-3.105995
C -3.267432 -2.290865 -0.72	²⁰⁴⁵⁶ C	0.347852	5.928558	-3.585461	Н	1.723971	-1.702658	-3.430816
C -3.039021 -2.920585 -1.99	⁹⁰⁹⁷⁸ C	0.509811	6.472799	-2.311942	Н	1.749645	0.088829	-3.277997
C -3.614129 -4.193461 -2.2	⁵⁴⁰⁵³ C	0.280141	5.684159	-1.181187	С	2.598365	-2.252390	0.565784
C -4.356687 -4.847223 -1.29	98233 H	0 409773	6 1 1 4 9 0 5	-0 190149	Ċ	1 537066	-2.982557	1 031119
C -4.545482 -4.251670 -0.02	28936 H	0.820259	7 507590	-2 194613	Ĥ	1 136909	-2.756666	2.017202
C -4.018338 -3.009948 0.25	51620 H	0.530277	6 536557	-4 467313	C	0 970974	-4 164015	0 299938
Н -4.166926 -2.574023 1.23	32245 н	-0.174923	4 163527	-4 711201	č	1 324616	-4 175018	-1 198406
Н -5.108742 -4.780479 0.73	34991 п	0.584425	2 773840	2 702250	C	2 145664	2 481417	0.751477
Н -4.785764 -5.822677 -1.5	09083 C	-0.384423	2.113049	-2.702339	U U	3.143004 4.097027	-2.40141/	-0./314//
H -3.442091 -4.647878 -3.2	26806 C	2 419040	2.050/0/	0.290604	П	4.08/05/	-1.991810	-0.980078
$C = 2.217746 = 2.275571 = 2.9^{\circ}$	53772 C	2.418949	1.991257	1.585454	U U	2.779745	-3./53614	-1.463979
C = 1.606638 = 1.080603 = 2.60	63463 C	3.520783	1.129859	1.630110	H	3.072332	-1.502/86	1.192463
H = 2.059432 = 2.752654 = 3.9	17429 C	3.959249	0.584001	2.843518	Н	1.133252	-5.168477	-1.619457
C = 2.059452 = -2.752054 = -5.9	$C_{05703}^{17423}$ C	3.304292	0.905357	4.030554	Н	0.657677	-3.476702	-1.721687
$C = \frac{1}{2}, \frac{9}{3}, \frac{3}{3}, \frac{9}{3}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{1}{2}, \frac{9}{3}, \frac{1}{2}, \frac{1}{2$	C 24001 C	2.208974	1.776542	4.003205	Н	2.969310	-3.662184	-2.538368
C = 1.88//10 = 0.11/104 = 1.36	C C	1.773855	2.311826	2.793445	Н	3.474205	-4.525254	-1.093554
0 -0.585/10 -0.055541 1.10	69590 H	0.922651	2.989721	2.783062	Н	-0.116506	-4.210162	0.440164
C = -2.058854 = 0.775066 = 2.85	54875 H	1.700741	2.044556	4.926490	Н	1.367788	-5.068152	0.793913
	Н	3.645468	0.487413	4.974033	Br	5.900850	-1.841849	0.732505
ĩ	С	-2.417327	1.535341	3.523615	С	0.306086	3.593389	1.165235
• A	C C	-2.417327 -3.480870	1.535341 2.034344	3.523615 2.725115	C H	0.306086 -0.369491	3.593389 3.544566	1.165235 0.311636
a for	C C C	-2.417327 -3.480870 -3.469547	1.535341 2.034344 1.791796	3.523615 2.725115 1.310678	C H H	0.306086 -0.369491 -0.105362	3.593389 3.544566 2.989805	1.165235 0.311636 1.977501
A	C C C	-2.417327 -3.480870 -3.469547 -4.511662	1.535341 2.034344 1.791796 2.368639	3.523615 2.725115 1.310678 0.531697	C H H H	0.306086 -0.369491 -0.105362 0.350146	3.593389 3.544566 2.989805 4.633096	1.165235 0.311636 1.977501 1.506652
XX	C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753	1.535341 2.034344 1.791796 2.368639 3.107602	3.523615 2.725115 1.310678 0.531697 1.117092	C H H H	0.306086 -0.369491 -0.105362 0.350146 2.319975	3.593389 3.544566 2.989805 4.633096 3.282337	1.165235 0.311636 1.977501 1.506652 1.733004
XX	C C C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642	C H H H C	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366
		-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296	C H H H C H	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710
	C C C C C C H	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559	С Н Н Н С Н Н	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004
	C C C C C C C H H	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227	С Н Н Н С Н Н	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029
	C C C C C C C C H H H	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064	С Н Н Н С Н Н Н	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933
	СССССНННН	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645	C H H C H H H H Cu	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515
C1 _{(S)-SN2p}	СССССНННН	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.885544 3.543858 2.233903 1.695025	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595	C H H H C H H H Cu Cu	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184
C1 _{(S)-SN2p}	C C C C C C C C H H H H H H H N	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940	C H H H C H H H C C H	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075
P 0.842322 0.569507 -0.15	С С С С С С С С С С С С С С С С С С С	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868	C H H H C H H H C U C H H	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.366335 2.306560 3.315554 1.763999	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489
P 0.842322 0.569507 -0.15 0 -0.216595 1.572237 -0.9	C C C C C C C C C C H H H H H H H H H S 55146 C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447 2.343985	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011 4.107601	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868 -0.223067	С Н Н Н Н С Н Н Н С С Н Н Н Н	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554 1.763999 2.423904	3.593389 3.54566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312 0.125610	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489 -3.701464
P 0.842322 0.569507 -0.15 O -0.216595 1.572237 -0.9 C -1.324948 0.921095 -1.5	C C C C C C C C C C C C C C C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447 2.343985 1.884338	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011 4.107601 4.139776	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868 -0.223067 -1.548349	С Н Н Н С Н Н Н С С Н Н Н С С Н Н Н С С Н Н С С Н Н Н С С Н Н Н С С И И И И	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554 1.763999 2.423904 0.293464	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312 0.125610 -3.238662	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489 -3.701464 -1.892078
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$\begin{array}{c c} \\ P & 0.842322 & 0.569507 & -0.15\\ O & -0.216595 & 1.572237 & -0.9\\ C & -1.324948 & 0.921095 & -1.5\\ C & -2.406724 & 0.617867 & -0.7\\ C & -3.488497 & -0.138892 & -1.2\\ C & -3.465282 & -0.435909 & -2.6\\ C & -4.537768 & -1.168168 & -3.2\\ C & -5.579794 & -1.627475 & -2.5\\ C & -5.582918 & -1.378568 & -1.1\\ C & -4.568924 & -0.654607 & -0.5\\ H & -4.58929 & -2.193116 & -2.9\\ H & -6.389769 & -1.768208 & -0.4\\ H & -6.389829 & -2.193116 & -2.9\\ H & -4.508601 & -1.372157 & -4.3\\ C & -2.355540 & -0.023309 & -3.4\\ C & -1.288002 & 0.618676 & -2.9\\ H & -2.348475 & -0.248490 & -4.5\\ C & -2.398665 & 1.023032 & 0.7\\ C & -1.331797 & 0.672163 & 1.5\\ \end{array}$	C C C C C C C C C C C C C C C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447 2.343985 1.884338 2.428410 3.437917 3.899371 3.354376 3.719310 4.685153 3.861243 2.064179 1.104861 3.350623 3.513238 4.375641 4.572776 3.908543 3.044567 2.854777	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011 4.107601 4.139776 5.039402 5.923955 5.902117 4.997816 4.986488 6.583441 6.622353 5.050114 3.451366 1.268534 0.033855 -1.019639 -2.088657 -2.125770 -1.081120 -0.014096	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868 -0.223067 -1.548349 -2.464370 -2.072421 -0.756779 0.158928 1.184347 -0.441050 -2.789328 3.488402 -1.859779 0.539213 1.433238 1.102955 1.983174 3.2551122 2.673423	СННННСННННССНННСССННССНННННННВР	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554 1.763999 2.423904 0.293464 0.037840 0.381688 1.280006 0.784177 2.115272 1.788392 2.058112 2.465673 1.036894 -0.813920 -0.356668 2.807025 2.697126 1.001446 -0.446353	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312 0.125610 -3.238662 -2.828176 -3.354215 -4.332991 -5.034005 -3.901609 -5.085438 -4.123446 4.648798 -5.816075 -2.189648 -2.885892 -3.374652 -5.646481 -2.583878 -4.588678 -4.588698 -1.014241	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489 -3.701464 -1.892078 -0.613171 0.555126 -2.245773 -2.930984 -2.812035 -1.003611 0.158694 1.026993 -0.681406 -0.400723 -2.690167 -0.141055 -1.249744 1.297673 1.621519 0.156297
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P 0.842322 0.569507 -0.15 O -0.216595 1.572237 -0.9 C -1.324948 0.921095 -1.5 C -2.406724 0.617867 -0.7 C -3.488497 -0.138892 -1.2 C -3.465282 -0.435909 -2.6 C -4.537768 -1.168168 -3.2 C -5.579794 -1.627475 -2.5 C -5.582918 -1.378568 -1.1 C -4.588627 -0.485693 0.5 H -4.583627 -0.485693 0.5 H -6.389769 -1.768208 -0.4 H -6.38929 -2.193116 -2.9 H -4.508601 -1.372157 -4.3 C -2.355540 -0.023309 -3.4 C -1.288002 0.618676 -2.9 H -2.348475 -0.248490 -4.5 C -2.398665 1.023032 0.77 C -1.331797 0.672163 1.5 O -0.219587 0.024264 1.0 C -1.354535 0.889342 2 94	C C C C C C C C C C C C C C C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447 2.343985 1.884338 2.428410 3.437917 3.899371 3.354376 3.719310 4.685153 3.861243 2.064179 1.104861 3.350623 3.513238 4.375641 4.572776 3.908543 3.044567 2.854277 4.060675	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011 4.139776 5.039402 5.923955 5.902117 4.997816 4.986488 6.583441 6.622353 5.050114 3.451366 1.268534 0.033855 -1.019639 -2.088657 -2.125770 -1.081120 -0.014986 -2.957019 0.809776	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868 -0.223067 -1.548349 -2.464370 -2.789328 1.184347 -0.441050 -2.789328 -3.488402 -1.589779 0.539213 1.433238 1.102955 1.983174 3.208184 3.550122 2.673432 3.891058	СННННСННННСОНННСОССННССНННННННН	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554 1.763999 2.423904 0.293464 0.037840 0.801688 1.280006 0.784177 2.115272 1.788392 2.058112 2.465673 1.036894 -0.356668 2.807025 2.697126 1.001446 -0.446353 4.904585 2.179162 5.2497120	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312 0.125610 -3.238662 -2.828176 -3.354215 -4.332991 -5.034005 -3.901609 -5.085438 -4.123446 -4.648798 -5.816075 -2.189648 -2.885892 -3.374652 -5.646481 -2.583878 -4.588698 -1.014241 0.790642 2.892920	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489 -3.701464 -1.892078 -0.613171 0.555126 -2.245773 -2.930984 -2.812035 -1.003611 0.158694 1.026993 -0.681406 -0.400723 -2.690167 -0.141055 -1.249744 1.297673 1.621519 0.156227 2.947771 1.724662
P         0.842322         0.569507         -0.15           0         -0.216595         1.572237         -0.9           0         -0.216595         1.572237         -0.9           0         -0.216595         1.572237         -0.9           0         -1.324948         0.921095         -1.5           0         -2.406724         0.617867         -0.7           C         -3.488497         -0.138892         -1.2           C         -3.465282         -0.435909         -2.6           C         -4.537768         -1.168168         -3.2           C         -5.579794         -1.627475         -2.5           C         -5.582918         -1.378568         -1.1           C         -4.568924         -0.654607         0.5           H         -6.389769         -1.768208         -0.4           H         -6.389769         -1.768208         -0.4           H         -6.389829         -2.193116         -2.9           H         -4.508001         -1.372157         -4.3           C         -2.355540         -0.023309         -3.4           C         -1.288002         0.618676         -2.9	C C C C C C C C C C C C C C C C C C C	-2.417327 -3.480870 -3.469547 -4.511662 -5.516753 -5.543955 -4.541492 -4.537097 -6.346206 -6.293664 -4.502952 -2.444594 1.916890 1.734447 2.343985 1.884338 2.428410 3.437917 3.354376 3.719310 4.685153 3.861243 2.064179 1.104861 3.350623 3.513238 4.375641 4.572776 3.908543 3.044567 2.854277 4.060675 -0.409486	1.535341 2.034344 1.791796 2.368639 3.107602 3.310141 2.784927 2.947688 3.888544 3.543858 2.233903 1.695025 1.719711 3.162011 4.107601 4.139776 5.039402 5.923955 5.902117 4.997816 4.986488 6.583441 6.622353 5.050114 3.451366 1.268534 0.033855 -2.125770 -1.081120 -0.014986 -2.957019 0.899765	3.523615 2.725115 1.310678 0.531697 1.117092 2.516642 3.299296 4.374559 2.966227 0.495064 -0.543645 4.598595 0.438940 0.811868 -0.223067 -1.548349 -2.464370 -2.072421 -0.756779 0.158928 1.184347 -0.441050 -2.789328 -3.488402 -1.859779 0.539213 1.433238 1.102955 1.983174 3.208184 3.550122 2.673432 3.891058 -3.471741	С Н Н Н Н С Н Н Н Н С С Н Н Н С С С С Н Н С С Н Н Н Н Н Н Н Н В Н Н Н .	0.306086 -0.369491 -0.105362 0.350146 2.319975 4.042343 3.654199 3.883374 5.122379 3.840845 1.356335 2.306560 3.315554 1.763999 2.423904 0.293464 0.037840 0.801688 1.280006 0.784177 2.115272 1.788392 2.058112 2.465673 1.036894 -0.813920 -0.356668 2.807025 2.697126 1.001446 -0.446353 4.904585 2.179162 5.248710 2.529222	3.593389 3.544566 2.989805 4.633096 3.282337 1.173069 0.346509 2.100649 1.038797 2.089241 -1.219390 -0.937544 -1.377413 -1.418312 0.125610 -3.238662 -2.828176 -3.354215 -4.332991 -5.034005 -3.901609 -5.085438 -4.123446 -4.648798 -5.816075 -2.189648 -2.885892 -3.374652 -5.646481 -2.583878 -4.588698 -1.014241 0.790642 -2.892869 -1.074421	1.165235 0.311636 1.977501 1.506652 1.733004 -0.827366 -1.429710 -1.381004 -0.700029 1.075933 -1.727515 -3.448184 -3.426075 -4.275489 -3.701464 -1.892078 -0.613171 0.555126 -2.245773 -2.930984 -2.812035 -1.003611 0.158694 1.026993 -0.681406 -0.400723 -2.690167 -0.141055 -1.249744 1.297673 1.621519 0.156227 2.947771 1.704603

			9	С	1.979158	2.516272	3.474193	С	3.954546	-0.013706	0.792763
	-	•	<b>A</b>	С	2.252594	3.640837	2.650636	Н	3.775581	0.654094	-0.049625
	<u>()</u>	1 <b>` ` ` ` ` `</b>	i i i i	С	1.826018	3.629426	1.280305	Н	3.410361	0.360125	1.663088
		$\sim$	ξ.J	С	2.182143	4.740371	0.465544	Н	5.024008	0.013171	1.026490
	· · · /	$-I \propto $	gr -	С	2.883077	5.808638	0.981532	Н	3.855132	-2.046340	1.375230
				С	3.265938	5.832694	2.342856	С	1.499990	-3.876264	-0.950268
G	S-X 19	- / <b>X</b> -9		С	2.958209	4.765878	3.155369	Н	0.544100	-3.551462	-1.371082
	1 19-0			Н	3.261957	4.760608	4.199439	Н	2.291714	-3.619201	-1.657554
	-0-0	$\mathbf{T}$	$\Gamma$	Н	3.811097	6.684941	2.738386	Н	1.477458	-4.966648	-0.849003
	- ° 7		$\sqrt{r}$	Н	3.148288	6.639343	0.333358	Н	2.726336	-3.662072	0.763091
	-	64	23	Н	1.906615	4.737236	-0.582558	Cu	-1.205349	-1.354330	-1.326052
	1.	SI _(S) -SN2p	3 3	Н	2.282042	2.540669	4.517826	С	-1.212031	-2.235887	-3.107425
		0 - 4 - 40 -		Ν	2.125458	-1.753130	0.276979	Η	-1.755874	-3.183614	-3.031226
Р	0.847239	-0.747695	-0.122116	С	3.587657	-1.468769	0.480849	Η	-1.683104	-1.609473	-3.870062
0	1.638514	0.393163	-1.047404	С	4.435128	-2.011802	-0.668580	Η	-0.168320	-2.425806	-3.383066
C	0.825504	1.447272	-1.475980	С	4.278779	-1.539323	-1.980474	С	-3.293985	-0.841031	-1.527239
C	0.515406	2.477328	-0.601102	С	5.089925	-2.021035	-3.007314	С	-2.814274	-0.001693	-0.463848
C	-0.416948	3.480171	-1.055442	С	6.072762	-2.979439	-2.741087	С	-2.941365	-0.405514	0.843441
C	-0.882232	3.446686	-2.414297	С	6.238356	-3.452723	-1.440028	С	-4.198633	-1.942158	-1.168820
C	-1.795283	4.43/639	-2.866093	С	5.422023	-2.970882	-0.412930	Н	-5.174043	-1.411109	-0.902513
C	-2.266864	5.40/529	-2.012542	Н	5.558403	-3.343604	0.600544	Н	-4.398715	-2.615528	-2.007536
C	-1.845572	5.418418	-0.662310	Н	6.998087	-4.198333	-1.221321	С	-3.757251	-2.690708	0.097912
C	-0.945499	4.484921	-0.19/015	Н	6.702682	-3.353219	-3.543630	С	-3.493516	-1.725634	1.270967
H	-0.645156	4.503864	0.843686	Н	4.956671	-1.646544	-4.018907	Н	-4.436710	-1.493452	1.786964
H	-2.243076	6.165/3/	0.018535	Н	3.516817	-0.795676	-2.193812	Н	-4.529757	-3.410346	0.386191
H	-2.9/408/	6.152365	-2.365568	С	1.791138	-3.218074	0.404234	Н	-2.430803	0.990436	-0.688900
Н	-2.128941	4.401233	-3.900135	С	0.749528	-3.489384	1.494831	Н	-3.375618	-0.403111	-2.517603
C	-0.448928	2.405228	-3.27/535	С	-0.299283	-4.400624	1.316626	Н	-2.823219	-2.178187	2.014745
0	0.368890	1.404/28	-2.8121/4	С	-1.183846	-4.689657	2.361041	Н	-2.844684	-3.265064	-0.124147
H C	-0./96413	2.394595	-4.30/248	С	-1.032859	-4.074300	3.602824	Н	-2.649377	0.288221	1.628408
C	1.099144	2.495555	0.770430	С	0.011733	-3.164803	3.794915	Br	-6.583607	-0.261661	0.489683
C	0.966284	1.380/0/	1.598992	С	0.890146	-2.878395	2.752451	Н	-0.434602	-4.899473	0.363054
0	0.354588	0.225810	1.155869	Н	-1.719034	-4.300553	4.414091	Н	1.695887	-2.166700	2.910951
C	1.369428	1.402026	2.955115	Н	0.682283	0.580861	-3.444613	Н	-1.990838	-5.398743	2.198097
				Н	1.173460	0.521348	3.558205	Н	0.142343	-2.681487	4.759550

#### 2.1.3. Quadrant diagrams

The elaboration of a quadrant diagram was attempted to correlate the geometrical properties of the chiral catalyst and the observed discrimination of the system. Indeed, even though the approach of the substrate was not the enantiodetermining step, we were convinced that this modelization would help us to apprehend the steric interactions at play during the key oxidative addition step. Thus, a rational model was designed from  $C1_{(R)-SN2p}$  and all potential approaches were subsequently implemented (figure 3). As mentioned in the manuscript, the rigid binaphthyl core and the upper phenyl part of the amine moiety were the most encumbering elements of the chiral catalyst and hence, logically shielded the quadrants II and IV of the model. In addition, the position of the transferable methyl group appeared to block the window III. Consequently, a single quadrant remained open to allow for the approach of both enantiomers of the racemic substrate, namely the quadrant I. With this model in hand, the substrate was superimposed in a way that facilitates the displacement of the leaving group in *anti*-S_N2^o or in *anti*-S_N2. Among the four possible routes, only two pathways allowed for the approach of the substrate by the open quadrant I. These possibilities were an *anti*-S_N2^o for

the *R*-enantiomer of the substrate and an *anti*- $S_N 2$  for its *S* antipode. Finally, such model conveniently explained the selectivity at play in the present process but we are confident with the fact that it could also provide an interesting tool for the rationalization of related reactions using a similar chiral catalyst.



Figure S3. Rationalization of the system by means of steric quadrant diagrams

## 2.2. Additional chemical experiments

### 2.2.1. Screening of various allylic derivatives

**Table S9.** Influence of the leaving group^(a)

X racemic substrate	CuTC (5 mol%) L1 (5.5 mo%) PhCH ₂ CH ₂ MgBr (1.1 CH ₂ Cl ₂ , -78°C	5 eq)	Ph (Ra)	$P^{h}(R)$ $P^{-N}$ $P^{O} P^{h}(R)$ $P^{O}(R)$ $P^{-1}(R)$
Entry	Х	Time (h)	Conversion (%) ^(b)	ee (%) ^(c)
1	OAc	15	70	0
2	OCO ₂ Me	15	83	4
3	OP(O)Ph ₂	3	> 99	8
4	OP(O)(OEt) ₂	3	> 99	14 ( <i>S</i> )
5	Cl	2	> 99	53 (S)
6	Br	1	> 99	78 ( <i>S</i> )
7	OTf	1	_(d)	_(d)

(a) Reaction conditions: the racemic substrate (0.5 mmol) was added to a solution of CuTC (5 mol%) and L1 (5.5 mol%) in  $CH_2Cl_2$  (2 ml). The reaction mixture was cooled to -78 °C, stirred for 10 min, and the Grignard reagent (1M in Et₂O, 1.5 eq) was added dropwise. The reaction mixture was stirred for the indicated period of time. (b) Conversion relative to the formation of 9, determined by ¹H NMR and GC-MS. (c) Determined by GC on chiral stationary phase after derivatization in corresponding diastereomeric mixture of epoxides. (d) The formation of 9 was not observed.

## 2.2.2. Evolution of the ee throughout the reaction



**Figure S4.** Monitoring of the *ee* of **6** and **9** during the course of the reaction (¹H NMR and GC on chiral stationary phase)

## 3. Experimental part

## **3.1. Preparation of allylic trifluoroacetates**

General procedure for the preparation of various cycloalk-2-en-1-yl 2',2',2'trifluoroacetates:

In a round-bottomed flask, a solution of cycloalkenol (1 eq) and triethylamine (2 eq) in dry diethylether (5 ml/mmol) was prepared and cooled to 0 °C. 2,2,2-trifluoroacetic anhydride (1.2 eq) was added followed by dimethylaminopyridine (0.05 eq), and the reaction mixture was stirred for 30 min at 0 °C. Then, the reaction mixture was warmed to room temperature and stirred for 2 h. The reaction was quenched with a solution of  $HCl_{aq}$  1M (5 ml/mmol) and extracted with diethylether (3x 5 ml/mmol). The organic layer was washed with a saturated solution of NaHCO_{3aq} (20 ml/mmol), dried over anhydrous Na₂SO₄, filtered and concentrated *in vacuo*. The crude mixture was distilled bulb-to-bulb to recover the desired allylic trifluoroacetate.



**Cyclohex-2-en-1-yl 2',2',2'-trifluoroacetate (6):** prepared from cyclohex-2en-1-ol. Purified by bulb-to-bulb distillation (50-60 °C, 0.5-1 mmHg). Yield = 46 %. Slightly yellow liquid.

 $\underbrace{^{1}\text{H NMR (400 MHz, CDCl}_{3}, 25 \text{ °C}):}_{1} \delta = 1.67 \text{-} 1.71 (M, 1H, CH_{2}), 1.75 \text{-} 1.80 (m, 1H, CH_{2}), 1.88 \text{-} 1.92 (m, 2H, CH_{2}), 2.01 \text{-} 2.05 (m, 1H, CH_{2}), 2.12 \text{-} 2.18 (m, 1H, CH_{2}), 5.43 (brs, 1H, CH), 5.74 \text{-} 5.77 (m, 1H, CH), 6.08 \text{-} 6.10 (m, 1H, CH) ppm.$ 

 $\frac{{}^{13}\text{C NMR (100 MHz, CDCl}_3, 25 \text{ °C}):}{110.5\text{-}119.0 (q, J = 284.4 Hz, CF_3), 123.2 (CH), 135.5 (CH), 156.9\text{-}158.0 (q, J = 35 Hz, C) ppm.}$ 

¹⁹F NMR (282 MHz, CDCl₃, 25 °C): δ = -75.3 (s, 3F, CF₃) ppm.



*cis*-5-methylcyclohex-2-en-1-yl 2',2',2'-trifluoroacetate (11): prepared from *cis*-5-methylcyclohex-2-enol (prepared from crotonaldehyde according to a reported procedure. *cis/trans* 12/1)⁷. Purified by bulb-to-bulb distillation (50-60 °C, 0.5-1 mmHg). Yield = 38 %. cis/trans = 12/1. Colorless liquid. The product was stored at -5 °C in the absence of light.

For *cis*-11 isomer:

<u>¹H NMR (400 MHz, CDCl₃, 25 °C)</u>:  $\delta$  = 1.02 (d, 3H, J = 6.6 Hz, CH₃), 1.43-1.49 (m, 1H, CH₂), 1.68-1.80 (m, 1H, CH₂), 1.82-1.95 (m, 1H, CH), 2.11-2.18 (m, 2H, CH₂), 5.56-5.63 (m, 2H, CH), 5.93-5.97 (m, 1H, CH) ppm.

 $\frac{{}^{13}\text{C NMR (100 MHz, CDCl}_3, 25 \text{ °C}):}{(CH), 110.4-118.9 (q, 1C, J = 286.0 Hz, CF_3), 124.5 (CH), 132.8 (CH), 156.9-158.1 (q, 1C, J = 41.9 Hz, C) ppm.}$ 

¹⁹F NMR (282 MHz, CDCl₃, 25 °C): δ = -75.3 (s, 3F, CF₃) ppm.



**Cyclopent-2-en-1-yl 2',2',2'-trifluoroacetate (12):** prepared from cyclopent-2en-1-ol. Purified by bulb-to-bulb distillation (30-40 °C, 0.5-1 mmHg). Yield = 28 %. Slightly yellow liquid. The product was stored at -25 °C in the absence of light.

<u>¹H NMR (400 MHz, CDCl₃, 25 °C)</u>: δ = 1.94-2.04 (m, 1H, CH₂), 2.32-2.45 (m, 2H, CH₂), 2.55-2.66 (m, 1H, CH₂), 5.87-5.89 (m, 2H, CH), 6.25-6.27 (m, 1H, CH) ppm.

¹³C NMR (100 MHz, CDCl₃, 25 °C):  $\delta$  = 29.5 (CH₂), 31.3 (CH₂), 85.5 (CH), 110.4-118.9 (q, 1C, J = 286.1 Hz, CF₃), 127.3 (CH), 140.7 (CH), 157.0-158.2 (q, 1C, J = 41.8 Hz, C) ppm. ¹⁹F NMR (282 MHz, CDCl₃, 25 °C):  $\delta$  = -75 2 (s, 3F, CF₃) ppm.

⁷ I. D. G. Watson, A. K. Yudin, J. Am. Chem. Soc. 2005, 127, 17516.

## 3.2. Alkylation products

## General procedure for the copper-catalyzed AAA of various cycloalk-2-en-1-yl 2',2',2'trifluoroacetates:

In a flame-dried Schlenk tube under argon atmosphere, CuTC (4.8 mg, 0.25 mmol, 0.10 eq) and L2 (15.1 mg, 0.028 mmol, 0.11 eq) were dissolved in dry dichloromethane (2 ml) and the solution was stirred for 10 min at room temperature. Then, the trifluoroacetate derivative (0.25 mmol) was added and the solution was cooled to -78 °C. After 10 min at this temperature, the organomagnesium reagent solution (1M in diethylether, 0.3 ml, 0.3 mmol, 1.2 eq) was added at a 0.6 ml/h rate and the reaction mixture was stirred for 3 h. The reaction was quenched with a solution of  $HCl_{aq}$  1M (8 ml) and extracted with diethylether (3x10 ml). The organic layer dried over anhydrous Na₂SO₄, filtered and concentrated *in vacuo*. The crude mixture was purified by chromatography on silica gel (pentane, R_f = 0.7) affording the desired alkylation product.

(*R*)-(2-(cyclohex-2-enyl)ethyl)benzene (9): prepared from cyclohex-2-en-1-yl 2',2',2',2'-trifluoroacetate (6). Yield = 85 %.  $ee_9$  = 97 %. Colorless liquid. The enantiomeric excess was determined by GC on a chiral stationary phase using Hydrodex B3P column, Method: 60-30-1-140-20-170-5, R_T = 102.17 (*S*), 102.76 (*R*) min. The enantiomeric excess was also determined after derivatization in corresponding mixture of diastereoisomeric epoxides using Hydrodex TBDM column, Method: 90-0-1-170-5, R_T = 71.97, 73.05, 76.61, 77.96 min.

¹<u>H NMR (400 MHZ, CDCl₃, 25 °C)</u>: δ = 1.27-1.36 (m, 1H, CH₂), 1.50-1.81 (m, 4H, CH₂),
1.84-1.90 (m, 1H, CH₂), 1.99-2.04 (m, 2H, CH₂), 2.08-2.18 (m, 1H, CH), 2.64-2.75 (m, 2H, CH₂), 5.64-5.68 (m, 1H, CH), 5.70-5.75 (m, 1H, CH), 7.18-7.23 (m, 3H, CH), 7.29-7.33 (m, 2H, CH) ppm.

 $\frac{{}^{13}\text{C NMR (100 MHZ, CDCl}_3, 25 \text{ °C}):}{34.9 (CH), 38.4 (CH_2), 125.8 (CH), 127.3 (C), 128.4 (2C, CH), 128.5 (2C, CH), 131.9 (CH), 143.0 (C) ppm.$ 

<u>IR (CHCl₃):</u> 71.9, 1453, 1493, 2856, 2923, 3023 cm⁻¹.

MS (EI mode) *m*/*z* (%): 186 (28), 143 (4), 129 (4), 104 (26), 91 (100), 65 (34), 53 (22).

<u>HRMS (EI)</u>: calculated for C₁₄H₁₈ [M⁺] 186.1407, found 186.1409.

<u>Optical activity:</u>  $[\alpha]^{25}_{D} = -72.5$  (c = 1.2 in CHCl₃, 92 % *ee*).



(*R*)-3-cyclopentylcyclohex-1-ene (13): prepared from cyclohex-2-en-1-yl 2',2',2'trifluoroacetate (6). Yield = 86 %.  $ee_{13}$  = 90 %. Colorless liquid. The enantiomeric excess was determined by GC on a chiral stationary phase after derivatization in corresponding mixture of diastereoisomeric epoxides using Hydrodex TBDM

column, Method: 60-0-1-170-5,  $R_T = 63.11, 63.21, 69.09, 70.73$  min

¹<u>H NMR (400 MHZ, CDCl₃, 25 °C)</u>:  $\delta = 1.14-1.28$  (m, 3H, CH₂), 1.46-1.62 (m, 6H, CH₂), 1.65-1.79 (m, 4H, CH₂), 1.86-1.90 (m, 1H, CH), 1.91-1.97 (m, 2H, CH₂), 5.67 (brs, 2H, CH) ppm.

¹³C NMR (100 MHZ, CDCl₃, 25 °C): δ = 21.9 (CH₂), 25.4 (CH₂), 25.5 (CH₂), 25.6 (CH₂), 28.6 (CH₂), 30.3 (CH₂), 30.8 (CH₂), 41.1 (CH), 45.8 (CH), 127.2 (CH), 131.5 (CH) ppm. <u>IR (CHCl₃)</u>: 720.9, 1217, 1228.9, 1365.8, 1447.7, 1738.8, 2865.6, 2947.2, 3021.2 cm⁻¹. <u>MS (EI mode) *m*/*z* (%)</u>: 150 (22), 135 (13), 121 (10), 108 (8), 93 (27), 79 (78), 67 (100). <u>HRMS (EI)</u>: calculated for C₁₁H₁₈ [M⁺] 150.1409, found 150.1391. <u>Optical activity</u>:  $[\alpha]^{25}_{D}$  = -80.6 (c = 1.0 in CHCl₃, 64 % *ee*).

For *trans*-14:

¹<u>H NMR (400 MHZ, CDCl₃, 25 °C)</u>: δ = 0.97 (d, 3H, J = 6.7 Hz, CH₃), 1.36-1.41 (m, 1H, CH₂), 1.53-1.57 (m, 1H, CH₂), 1.60-1.73 (m, 3H, CH₂), 1.79-1.88 (m, 1H, CH), 2.09-2.18 (m, 2H, CH₂ and CH), 2.65-2.71 (m, 2H, CH₂), 5.66-5.72 (brs, 2H, CH), 7.18-7.24 (m, 3H, CH), 7.28-7.32 (m, 2H, CH) ppm.

 $\frac{{}^{13}\text{C NMR (100 MHZ, CDCl}_3, 25 \text{ °C}):}{(CH_2)} \delta = 21.6 (CH_3), 24.8 (CH), 33.4 (CH), 33.8 (CH_2), 33.9 (CH_2), 35.8 (CH_2), 38.1 (CH_2), 125.7 (CH), 126.4 (CH), 128.4 (2C, CH), 128.5 (2C, CH), 131.0 (CH), 143.0 (C) ppm.$ 

For *cis*-14:

¹<u>H NMR (400 MHZ, CDCl₃, 25 °C)</u>:  $\delta$  = 0.98 (m, 1H, CH₂), 1.01 (d, 3H, J = 6.3 Hz, CH₃), 1.55-1.68 (m, 4H, CH₂), 1.81-1.87 (brs, 1H, CH₂), 2.04-2.11 (brs, 1H, CH₂), 2.18-2.26 (m, 1H, CH), 2.64-2.74 (m, 2H, CH₂), 5.61-5.65 (m, 1H, CH), 5.71-5.75 (m, 1H, CH), 7.18-7.24 (m, 3H, CH), 7.28-7.33 (m, 2H, CH) ppm.

 $\frac{{}^{13}\text{C NMR (100 MHZ, CDCl}_3, 25 \text{ °C}):}{36.3 (CH), 38.6 (CH_2), 38.7 (CH_2), 125.7 (CH), 126.9 (CH), 128.4 (2C, CH), 128.5 (2C, CH), 131.7 (CH), 143.0 (C) ppm.$ 

For the mixture of isomers:

<u>IR (CHCl₃):</u> 700, 746.7, 1216.9, 1229, 1374.5, 1454.7, 1496.3, 1739, 2906, 2947.3 cm⁻¹.

<u>MS (EI mode) *m*/z (%):</u> 200 (29), 172 (5), 143 (8), 122 (50), 109 (27), 104 (52), 91 (100), 79 (30), 67 (73).

<u>HRMS (EI)</u>: calculated for  $C_{15}H_{20}$  [M⁺] 200.1565, found 200.1568.

(*R*)-(2-(cyclopent-2-enyl)ethyl)benzene (15): prepared from cyclopent-2-en-1-yl 2',2',2'-trifluoroacetate (12) directly after distillation. Yield = 78 %.  $ee_{15} = 62$  %. Colorless liquid. The enantiomeric excess was determined by GC on a chiral stationary phase after derivatization in corresponding mixture of diastereoisomeric epoxides using Hydrodex TBDM column, Method: 60-0-1-170-5, R_T = 90.41, 90.93, 97.62, 99.06 min. ¹<u>H NMR (400 MHZ, CDCl₃, 25 °C)</u>:  $\delta = 1.44$ -1.53 (m, 1H, CH₂), 1.58-1.67 (m, 1H, CH₂), 1.72-1.81 (m, 1H, CH₂), 2.06-2.15 (m, 1H, CH₂), 2.26-2.45 (m, 2H, CH₂), 2.63-2.73 (m, 3H, CH₂), 5.72-5.78 (m, 2H, CH), 7.18-7.24 (m, 3H, CH), 7.28-7.33 (m, 2H, CH) ppm.

 $\frac{{}^{13}\text{C NMR (100 MHZ, CDCl}_{\underline{3}}, 25 \text{ °C}):}{45.3 (CH), 125.7 (CH), 128.4 (2C, CH), 128.5 (2C, CH), 130.0 (CH), 135.0 (CH), 142.9 (C) ppm.$ 

<u>IR (CHCl₃):</u> 697.7, 717.5, 748.6, 772.2, 1362.2, 1454.2, 1496, 1739.1, 2850.5, 2929.9, 30.26.9, 3050.9 cm⁻¹.

<u>MS (EI mode) *m*/z (%):</u> 172 (28), 152 (2), 144 (8), 129 (4), 115 (4), 104 (36), 92 (88), 81 (44), 67 (100), 53 (14), 51 (18).

<u>HRMS (EI)</u>: calculated for  $C_{13}H_{16}$  [M⁺] 172.1249, found 172.1252.

<u>Optical activity:</u>  $[\alpha]^{25}_{D} = -52$  (c = 1.5 in CHCl₃, 44 % *ee*).



# 4. Spectroscopic and chromatographic data





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