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ELECTRONIC SUPPLEMENTARY INFORMATION

Changing aromatic properties through stacking: the faceto-face dimer of Ni(II) bis(pentafluorophenyl)norcorrole[†]

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S1 Molecular orbitals



Fig. S1 The LUMO of the monomer (left) and the HOMO of the monomer (right)



Fig. S2 The LUMO+1 of the dimer (left) and the LUMO of the dimer (right)



Fig. S3 The HOMO of the dimer (left) and the HOMO-1 of the dimer (right)

Table S1 Orbital energies (in eV) of the monomer and the dimer calculated at the CAM-B3LYP/def2-TZVP level as well as the irreducible representations (IRREP) of the frontier orbitals of the dimer, which belongs to the C_{2h} point group. The total energies of the monomer and dimer are -3873.90393 a.u. and -7747.83695 a.u., which yield a binding energy of 76.4 kJ/mol.

orbital energy (eV)	Monomer	Dimer	IRREP
LUMO+1		-2.972	B_u
LUMO	-3.047	-3.320	A_u
HOMO	-6.484	-5.939	A_g
HOMO-1		-6.205	B_g

S2 Molecular structure of the dimer



Fig. S4 The molecular structure of 1_2 seen from the side, which reveals the parallel orientation of the pentafluorophenyl substituents. The brown atoms are carbon, the blue ones are nitrogen, the nickel atoms are grey, and the hydrogen are pink. Two of the pentafluorophenyl substituents are marked with yellow crosses. The picture has been made with Vesta.⁹



Fig. S5 The positions of the integration planes of 1 for determining the strength of the current-density pathways are shown with the colored lines in the upper-left picture. The current density is calculated at the CAM-B3LYP/def2-TZVP level. The three other pictures show the calculated ring-current profiles. The color of the frame around them matches the color of the integration plane in the upper left picture. The pictures have been made with Origin? and PowerPoint.



Fig. S6 The positions of the integration planes of 1_2 for determining the strength of the current-density pathways are shown with the colored lines in the upper-left picture. The current density is calculated at the CAM-B3LYP/def2-TZVP level. The three other pictures show the calculated ring-current profiles. The color of the frame around them matches the color of the integration plane in the upper left picture. The pictures have been made with Origin? and PowerPoint.



Fig. S7 The ring-current profile of 1' passing through the red plane. The current density is calculated at different levels of theory. The pentafluorophenyl substituents are replace with hydrogen atoms.



Fig. S8 The ring-current profile of $1'_2$ passing through the red plane. The current density is calculated at different levels of theory. The pentafluorophenyl substituents are replace with hydrogen atoms.



Fig. S9 The upper left picture is the top view of the current density crossing the plane which is perpendicular the external magnetic field as shown in the upper right picture. The four strong red spots are due to the adjacent H atoms. The lower right picture shows the current density passing a plane in the middle of 1_2 . The magnetic field is from above parallel to the plane. The same plane is shown as side view in the lower left picture. The pictures has been made with Paraview?

S4 Electron density



Fig. S10 The electron density of $\mathbf{1}_2.$ The electron density between the two Ni atoms is seen.

S5 Isotropic nuclear magnetic shielding constants

S5.1 Monomer

Monomer 1H NMR shielding constants in beta position

Level	Average	H19	H21	H28	Н32
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP	30.974303 29.844912 29.351458 29.002611 28.274654 28.337066 31.112409	30.858047 29.654736 29.178386 28.819628 27.921137 28.066465 31.246931	31.069241 30.008080 29.500103 29.161281 28.594187 28.579962 30.978735	31.097967 30.029742 29.516093 29.175052 28.602199 28.580048 31.000035	30.865421 29.679327 29.203741 28.846870 27.972123 28.112918 31.220486
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Monomer 1H NMR shielding constants in beta position

Level	H38	H43	H47	H50
B3LYP/TZVP	31.068962	30.869518	31.098146	30.867118
BHLYP/TZVP	30.007399	29.682879	30.029657	29.667479
CAM-B3LYP/TZVP	29.499614	29.207357	29.515570	29.190796
wB97X-D/TZVP	29.160813	28.850511	29.174461	28.832271
HF/TZVP	28.593320	27.973590	28.601496	27.939176
HF/SVP	28.579359	28.115478	28.578843	28.083458
MP2/SVP	30.978676	31.225625	30.999358	31.249424
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Monomer 61Ni NMR shielding constants

	Ni
B3LYP/TZVP	-4352.584550
BHLYP/TZVP	-7242.372009
CAM-B3LYP/TZVP	-4650.449617
wB97X-D/TZVP	-4772.027240
HF/TZVP	-14608.279269
HF/SVP	-14054.967261
MP2/SVP	2797.108328
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Monomer 13C NMR shielding constants in beta position next to the direct link between the pyrrole rings $% \left({{{\left[{{{\rm{D}}_{\rm{T}}} \right]}}} \right)$

Level	Average	C20	C27	C37	C46
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/TZVP HF/SVP MP2/SVP	66.031905 69.273729 67.224395 69.645828 78.004785 88.747752 93.762020	65.938668 69.206393 67.170318 69.598012 77.991878 88.735640 93.616816	66.118262 69.334067 67.270423 69.685051 78.011017 88.747041 93.898151	65.945586 69.212684 67.181597 69.609716 78.003501 88.750418 93.607028	66.125102 69.341773 67.275243 69.690533 78.012744 88.757909 93.926083

Monomer 13C NMR shielding constants in beta position next to the meso link between the pyrrole rings

Level	Average	C18	C31	C42	C49
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/TZVP HF/SVP MP2/SVP	48.175593 46.218602 46.042281 49.006877 45.897014 59.073237 86.781389	48.261886 46.250518 46.074708 49.031052 45.813432 59.013079 86.966208	48.057676 46.157665 45.979860 48.951925 45.951305 59.120616 86.599733	48.064162 46.141392 45.966890 48.940861 45.881036 59.042750 86.617879	48.318649 46.324831 46.147667 49.103669 45.942284 59.116501 86.941735

Monomer 15N NMR shielding constants of the nitrogen atoms $% \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NM$

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Level	Average(9,	,10) N9	N10
B3LYP/TZVP	-16.680038	-16.698169	-16.661907
BHLYP/TZVP	1.669926	1.648914	1.690937
CAM-B3LYP/TZVP	-7.448288	-7.467070	-7.429505
wB97X-D/TZVP	-3.208477	-3.225564	-3.191389
HF/TZVP	31.596737	31.559056	31.634418
HF/SVP	55.167424	55.119375	55.215472
MP2/SVP	36.475950	36.521520	36.430380

Monomer 15N NMR shielding constants of the nitrogen atoms

Level	Average(1	2,16) N12	N16	Average(9,10,12,16)
B3LYP/TZVP	-14.702983	-14.697041	-14.708924	-15.691511
BHLYP/TZVP	3.378677	3.387175	3.370178	2.524302
CAM-B3LYP/TZVP	-5.686155	-5.673852	-5.698457	-6.567222
wB97X-D/TZVP	-1.496954	-1.481878	-1.512029	-2.352716
HF/TZVP	32.961314	32.958521	32.964107	32.279026
HF/SVP	56.422355	56.425893	56.418816	55.794890
MP2/SVP	37.967337	37.98748	37.947193	37.221644

S5.2 Monomer without pentafluorophenyl groups

Monomer 1H NMR shielding constants in beta position

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Level	Average	Н9	H11	H17	H20
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP	30.553719 29.381975 28.984064 28.665827 27.937050 27.922430 30.180891	30.253060 28.993586 28.624983 28.304313 27.375640 27.448429 30.093267	30.850568 29.766352 29.340204 29.024886 28.494279 28.392464 30.268147	30.895842 29.805246 29.374230 29.056704 28.522839 28.416728 30.304807	30.215404 28.962466 28.596552 28.277134 27.354902 27.431463 30.057136
CASSCF/TZVP 14/14	26.8919 ========	26.2772	27.5018 ========	27.5204 ========	26.2675

Monomer 1H NMR shielding constants in beta position

Level	H25	H28	H31	нзз
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP CASSCF/TZVP 14/14	30.850177 29.766070 29.340178 29.024825 28.494221 28.392238 30.266422 27.5031	30.215437 28.961978 28.596066 28.276702 27.353003 27.430057 30.059464 26.2656	30.900169 29.809293 29.377788 29.060145 28.526428 28.420366 30.308990 27.5219	30.249095 28.990812 28.622511 28.301908 27.375090 27.447695 30.088898 26.2775

Monomer 61Ni NMR shielding constants

	 Ni
B3LYP/TZVP	-4347.946257
BHLYP/TZVP	-7218.463850
CAM-B3LYP/TZVP	-4642.442260
wB97X-D/TZVP	-4764.158895
HF/TZVP	-14555.781068
HF/SVP	-13978.731505
MP2/SVP	2742.411109
CASSCF/TZVP 14/14	-7684.2286

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Monomer 13C NMR shielding constants in beta position next to the direct link between the pyrrole rings $% \left({{\left[{{{\rm{NMR}}} \right]}_{\rm{A}}} \right)$

Level	Average	C10	C16	C24	C30
B3LYP/TZVP	67.192170	67.013585	67.356646	67.006755	67.391695
BHLYP/TZVP	70.565611	70.433245	70.682372	70.431636	70.715190
CAM-B3LYP/TZVP	68.421043	68.300556	68.526333	68.303448	68.553835
wB97X-D/TZVP	70.754916	70.646808	70.848922	70.650324	70.873611
HF/TZVP	79.380764	79.312492	79.431468	79.319967	79.459128
HF/SVP	90.230143	90.177369	90.266388	90.184347	90.292467
MP2/SVP	95.213084	95.073240	95.343237	95.060203	95.375656
CASSCF/TZVP 14/14	81.9022	81.8575	81.9328	81.8763	81.9423

Monomer 13C NMR shielding constants in beta position next to the meso link between the pyrrole rings $% \left({{{\left[{{{\rm{NMR}}} \right]}_{\rm{A}}}_{\rm{A}}} \right)$

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Level	Average	C8	C19	C27	C32
B3LYP/TZVP	48.072852	48.350046	47.804130	47.810389	48.326844
BHLYP/TZVP	46.322840	46.534583	46.118037	46.108104	46.530636
CAM-B3LYP/TZVP	45.905531	46.117849	45.701908	45.690572	46.111796
wB97X-D/TZVP	48.846146	49.045024	48.655062	48.644232	49.040265
HF/TZVP	46.753580	46.488034	47.804130	46.197985	46.524171
HF/SVP	59.367038	59.482446	59.257947	59.215131	59.512629
MP2/SVP	85.585348	85.821802	85.352467	85.382846	85.784277
CASSCF/TZVP 14/14	47.8902	47.9757	47.8153	47.7824	47.9872
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Monomer 15N NMR shielding constants of the nitrogen atoms

Level	Average(2,3)	N2	N3
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP WB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP	-15.568332 2.910113 -6.662562 -2.657330 31.956750 56.356064	-15.557844 2.917094 -6.654002 -2.648540 31.949431 56.346214	-15.578820 2.903132 -6.671122 -2.666120 31.964068 56.365914
CASSCF/TZVP 14/14	36.3585	36.4352	36.2818

Monomer 15N NMR shielding constants of the nitrogen atoms

B3LYP/TZVP -13.603580 -13.600595 -13.606565 -14.585956 BHLYP/TZVP 4.660326 4.673662 4.646990 3.785220 CAM-B3LYP/TZVP -4.869064 -4.855319 -4.82808 -5.765812 wB97X-D/TZVP -0.924111 -0.911469 -0.936753 -1.790721 HF/TZVP 33.402190 33.418477 33.385902 32.679470	Level	Average(5,6)	N5	N6	Average(2,3,5,6)
HF/SVP57.70431357.71721257.69141457.030189MP2/SVP42.19750842.22304442.17197141.374509CASSCF/TZVP 14/1437.959438.063237.855537.1590	B3LYP/TZVP	-13.603580	-13.600595	-13.606565	5 -14.585956
	BHLYP/TZVP	4.660326	4.673662	4.646990	3.785220
	CAM-B3LYP/TZVP	-4.869064	-4.855319	-4.882808	3 -5.765812
	wB97X-D/TZVP	-0.924111	-0.911469	-0.936753	3 -1.790721
	HF/TZVP	33.402190	33.418477	33.385902	2 32.679470
	HF/SVP	57.704313	57.717212	57.691414	4 57.030189
	MP2/SVP	42.197508	42.223044	42.171971	41.374509
	CASSCF/TZVP 14/14	37.9594	38.0632	37.8555	37.1590

S6 Free-base norcorrole

Monomer 1H NMR shielding constants in beta position

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Level	Average	Н6	H7	H25	H26
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP	28.978886 28.981343 27.654660 27.439136	28.995852 28.998500 27.727797 27.529794	28.246303 28.250225 26.914424 26.696939	29.094575 29.096133 27.755056 27.529144	28.995850 28.998506 27.727797 27.529794

HF/TZVP		26.986395	27.170892	26.032549	27.144952	27.170892
HF/SVP		26.988906	27.086590	26.134623	27.146889	27.086590
MP2/SVP		28.319314	28.158226	27.861681	28.478966	28.158226
CASSCF/TZVP	12/11	26.1149	26.0240	25.3053	26.6883	26.0300
CASSCF/TZVP	12/12	26.6483	26.6985	26.1987	26.9335	26.6985
CASSCF/TZVP	16/16	26.8267	26.7249	26.2282	27.1992	26.7249
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Monomer 1H NMR shielding constants in beta position

 Level	H27	========= H28	н29	нзо
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/TZVP MP2/SVP CASSCF/TZVP 12/11 CASSCF/TZVP 12/12 CASSCF/TZVP 12/12 CASSCF/TZVP 16/16	29.094574 29.096138 27.755056 27.529144 27.144952 27.14689 28.478966 26.4060 26.9335 27.1992	29.578816 29.580504 28.221362 28.000666 27.597185 27.587522 28.778383 26.5787 26.7626 27.1546	28.246303 28.250228 26.914424 26.696939 26.032549 26.134623 27.861681 25.3265 26.1987 26.2282	29.578816 29.580510 28.221362 28.000666 27.597185 27.587522 28.778383 26.5601 26.7626 27.1546

Monomer 13C NMR shielding constants in beta position next to the direct link between the pyrrole rings $% \left({{\left[{{{\rm{NMR}}} \right]}_{\rm{A}}} \right)$

Level	Average	C4	C20	C22	C24
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP CASSCF/TZVP 12/11 CASSCF/TZVP 12/12 CASSCF/TZVP 16/16	67.185208 67.234007 67.466256 70.026032 76.095458 87.360310 96.573796 71.9308 77.5176 83.0996	64.343280 64.393581 63.596812 66.030322 71.363501 82.526148 92.643947 63.8589 77.5187 77.5308	64.343227 64.393677 63.596815 66.030320 71.363501 82.526148 92.643947 64.0101 77.5187 77.5308	$\begin{array}{c} 70.027170\\ 70.074344\\ 71.335696\\ 74.021742\\ 80.827414\\ 92.194472\\ 100.503645\\ 79.2906\\ 77.5165\\ 88.6684 \end{array}$	$\begin{array}{c} 70.027153\\ 70.074425\\ 71.335700\\ 74.021743\\ 80.827416\\ 92.194472\\ 100.503645\\ 80.5634\\ 77.5165\\ 88.6684 \end{array}$

Monomer 13C NMR shielding constants in beta position next to the meso link between the pyrrole rings

Level	Average	C5	C19	C21	C23
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP CASSCF/TZVP 12/11 CASSCF/TZVP 12/12 CASSCF/TZVP 16/16	$50.465969 \\ 50.476513 \\ 48.905438 \\ 51.727890 \\ 53.761489 \\ 66.156681 \\ 86.863554 \\ 59.4681 \\ 69.6298 \\ 73.6851$	44.593662 44.600853 40.981810 43.708200 41.520280 55.294544 82.687380 42.5946 61.7331 62.0098	56.338269 56.352165 56.829064 59.747579 66.002698 77.018817 91.039727 79.7859 77.5264 85.3604	56.338266 56.352185 56.829066 59.747581 66.002699 77.018817 91.039727 72.4654 77.5264 85.3604	$\begin{array}{c} 44.593677\\ 44.600848\\ 40.981810\\ 43.708199\\ 41.520280\\ 55.294544\\ 82.687380\\ 43.0265\\ 61.7331\\ 62.0098 \end{array}$

Monomer 15N NMR shielding constants of the nitrogen atoms with ${\rm H}$

Level	Average	N8	N11
B3LYP/TZVP BHLYP/TZVP	17.504962 7.4584270	17.504975 17.458406	17.504949 17.458448
CAM-B3LYP/TZVP	24.942908	24.942907	24.942908
HF/TZVP	42.239055	42.239055	42.239054
HF/SVP	62.389080	62.389080	62.389080

MP2/SVP		70.047162	70.047162	70.047162
CASSCF/TZVP	12/11	60.4821	66.7636	54.2006
CASSCF/TZVP	12/12	63.3141	63.3141	63.3140
CASSCF/TZVP	16/16	74.7043	74.7043	74.7043

Monomer 15N NMR shielding constants of the nitrogen atoms without ${\rm H}$

Level	Average	N1	N10	
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B3LYP/TZVP	-79.369598	-79.369600	-79.369596	
BHLYP/TZVP	-79.344160	-79.344194	-79.344126	
CAM-B3LYP/TZVP	-74.049059	-74.049061	-74.049057	
wB97X-D/TZVP	-69.765399	-69.765400	-69.765397	
HF/TZVP	-66.010815	-66.010817	-66.010813	
HF/SVP	-44.353409	-44.353409	-44.353409	
MP2/SVP	-12.224169	-12.224169	-12.224169	
CASSCF/TZVP 12/11	-40.0573	-40.6059	-39.5087	
CASSCF/TZVP 12/12	-55.2609	-55.2609	-55.2609	
CASSCF/TZVP 16/16	-53.6272	-53.6272	-53.6272	

S6.1 Dimer

Dimer 1H NMR shielding constants in beta position

Level	Average	H19	H21	H28	H32
B3LYP/TZVP	24.203882	24.365794	23.948604	24.074892	24.426238
BHLYP/TZVP	23.936320	24.148082	23.614887	23.807206	24.175105
CAM-B3LYP/TZVP	23.934371	24.132801	23.636570	23.791528	24.176585
wB97X-D/TZVP	23.965894	24.159637	23.674249	23.825719	24.203971
HF/TZVP	24.012204	24.284516	23.616915	23.889364	24.258022
HF/SVP	24.216070	24.472197	23.841185	24.128844	24.422053

Dimer 61Ni NMR shielding constants

B3LYP/TZVP -4188.607224		Ni
BHLYP/TZVP -6784.455429 CAM-B3LYP/TZVP -4454.990422 wB97X-D/TZVP -4596.989650 HF/TZVP -13497.920895 HF/SVP -12921.709049	B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/TZVP	-4188.607224 -6784.455429 -4454.990422 -4596.989650 -13497.920895 -12921.709049

Dimer 13C NMR shielding constants in beta position next to the direct link between the pyrrole rings $% \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NM$

Level	C20	C27	Average
B3LYP/TZVP	53.985845	55.639488	54.812667
BHLYP/TZVP	55.541490	57.622553	56.582022
CAM-B3LYP/TZVP	53.584623	55.559253	54.571938
wB97X-D/TZVP	56.158824	58.226628	57.192726
HF/TZVP	60.580728	63.282022	61.931375
HF/SVP	72.305775	75.022248	73.664008
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Dimer 13C NMR shielding constants in beta position next the meso link between the pyrrole rings $% \left({{{\rm{D}}_{\rm{T}}}} \right)$

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Level	C18	C31	Average
B3LYP/TZVP	51.082684	48.413415	49.748050

BHLYP/TZVP	51.932374	48.931247	50.431811
CAM-B3LYP/TZVP	50.885271	47.869700	49.377486
wB97X-D/TZVP	53.656153	50.647205	52.151679
HF/TZVP	56.422596	53.118551	54.770574
HF/SVP	67.661519	64.900002	66.280761

Dimer 15N NMR shielding constants of the nitrogen atoms $% \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}$

Level	N9	N12	Average
B3LYP/TZVP	35.526985	32.984273	34.255629
BHLYP/TZVP	54.498968	50.461952	52.480460
CAM-B3LYP/TZVP	41.954971	38.680915	40.317943
wB97X-D/TZVP	44.410606	41.243016	42.826811
HF/TZVP	87.527639	81.613117	84.570378
HF/SVP	107.986332	103.033408	105.509870

S6.2 Dimer without pentafluorophenyl groups

Dimer 1H NMR shielding constants in beta position

B3LYP/TZVP24.15979324.45245223.87102924.16685224.148837BHLYP/TZVP23.90626424.36579423.94860424.07489224.426238CAM-B3LYP/TZVP23.90072924.22433223.57795223.90803923.892594wB97X-D/TZVP23.92996324.24338123.61546523.93859123.922413HF/TZVP24.15979324.45245223.87102924.16685224.148837HF/SVP24.25660024.64688923.85229924.29181724.235394MP2/SVP24.12181524.37524123.86348624.07551924.173013CASSCF/SVP14/1424.160124.529923.774124.150324.1860	Level	Average	Н9	H11	H17	H20
	B3LYP/TZVP	24.159793	24.452452	23.871029	24.166852	24.148837
	BHLYP/TZVP	23.906264	24.365794	23.948604	24.074892	24.426238
	CAM-B3LYP/TZVP	23.900729	24.224332	23.577952	23.908039	23.892594
	wB97X-D/TZVP	23.929963	24.24381	23.615465	23.938591	23.922413
	HF/TZVP	24.159793	24.452452	23.871029	24.166852	24.148837
	HF/SVP	24.256600	24.646889	23.852299	24.291817	24.235394
	MP2/SVP	24.121815	24.375241	23.863486	24.075519	24.173013
	CASSCF/SVP 14/14	24.1601	24.5299	23.7741	24.1503	24.1860

Dimer 61Ni NMR shielding constants

	Ni
B3LYP/TZVP	-4164.004090
BHLYP/TZVP	-6778.177746
CAM-B3LYP/TZVP	-4444.092310
wB97X-D/TZVP	-4584.654044
HF/TZVP	-13495.813469
HF/SVP	-12918.680881
MP2/SVP	2885.550824
CASSCF/SVP 14/14	-11463.5570

Dimer 13C NMR shielding constants in beta position next to the direct link between the pyrrole rings

Level	C10	C16	Average
B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/TZVP MP2/SVP CASSEE (SVP 14/14	55.377785 57.121683 55.051095 57.518063 55.377785 73.933327 88.142859 72.560	56.822350 59.028509 56.826535 59.355701 56.822350 76.260719 89.688051 77.2007	56.100068 58.075096 55.938815 58.436882 56.100068 75.097023 88.915455 74.2904
	10.0000	10.2001	11.0001

Dimer 13C NMR shielding constants in beta position next to the meso link between the pyrrole rings $% \left(\frac{1}{2} \right) = 0$

Level	C8	C19	Average
B3LYP/TZVP	53.938477	49.741892	51.840185
BHLYP/TZVP	54.927689	50.381870	52.654780
CAM-B3LYP/TZVP	53.601067	49.090175	51.345621
wB97X-D/TZVP	56.186480	51.740098	53.963289
HF/TZVP	53.938477	49.741892	51.840185
HF/SVP	71.054319	66.173414	68.613867
MP2/SVP	86.408773	83.110249	84.759511
CASSCF/SVP 14/14	70.0004	66.1298	68.0651

Dimer 15N NMR shielding constants of the nitrogen atoms $% \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}}} \right) = \left({{{\rm{NMR}}$

LevelN2N5AverageB3LYP/TZVP35.91344932.71529334.314371BHLYP/TZVP54.79661950.12745152.462035CAM-B3LYP/TZVP42.14300738.32922440.236116wB97X-D/TZVP44.54838940.87284042.710615HF/TZVP35.91344932.71529334.314371HF/SVP107.717453102.266843104.992148MP2/SVP80.42315677.94253579.182846CASSCF/SVP14/14102.962697.4731100.2179	=======================================				==
B3LYP/TZVP35.91344932.71529334.314371BHLYP/TZVP54.79661950.12745152.462035CAM-B3LYP/TZVP42.14300738.32922440.236116wB97X-D/TZVP44.54838940.87284042.710615HF/TZVP35.91344932.71529334.314371HF/SVP107.717453102.266843104.992148MP2/SVP80.42315677.94253579.182846CASSCF/SVP14/14102.962697.4731100.2179	Level	N2	N5	Average	
	B3LYP/TZVP BHLYP/TZVP CAM-B3LYP/TZVP wB97X-D/TZVP HF/TZVP HF/SVP MP2/SVP CASSCF/SVP 14/14	$\begin{array}{c} 35.913449\\ 54.796619\\ 42.143007\\ 44.548389\\ 35.913449\\ 107.717453\\ 80.423156\\ 102.9626 \end{array}$	32.715293 50.127451 38.329224 40.872840 32.715293 102.266843 77.942535 97.4731	34.314371 52.462035 40.236116 42.710615 34.314371 104.992148 79.182846 100.2179	

S7 Cartesian coordinates of the molecular structures

Monomer or 1

Ni	1 7345550	0 2053831	-0 1680936
	111010000	0.2000001	0.1000000
F	6.4598840	-1.3871514	-2.2698142
-	0 000 1000	0 0070704	0.00004.00
F	6.3834863	-0.2270764	2.2826189
F	0 0026696	0 7011052	2 4662008
г	9.0030000	-0.7911955	2.4002900
F	10 3591021	-1 6568608	0 2893632
-	10.0001021	1.0000000	0.2000002
F	9.0796649	-1.9538618	-2.0777384
-	0 4457500	4 0000000	0 0500070
F	-2.115/530	1.8290029	3.0562672
F	2 5156106	0 0075601	1 2165070
г	-3.5150120	0.02/5001	-1.5165970
N	3 2040829	1 2264695	-0 3333216
14	0.2040020	1.2204000	-0.0000210
Ν	0.8532261	1.7699155	-0.1117331
~	1 0000000	0 4700074	0.4440000
C	4.8896229	-0.4/860/1	-0.1112682
N	0 28603/5	0 7055303	0 1068800
14	0.2009345	-0.1900090	0.1908809
F	-6 0416672	1 4473436	-0 6454036
-	0.0110012	1.11/0100	0.01010000
F	-6.6130195	2.2636504	1.8716691
~	0.0701100	0.0001.000	1 0000000
C	8.3/61126	-0.9331622	1.3090200
N	2 6406507	1 3308888	0 0234606
14	2.0400307	-1.5550000	-0.0234000
С	0.4944385	-2.0752463	0.4792742
ä	0 5500470	0.4400700	0.0070700
С	-0.5539479	3.4483738	0.2870792
TT	1 4500506	4 0100224	0 5002004
п	-1.4500526	4.0100334	0.5005924
С	2.8775927	-3,4558782	0.6094077
	2.0.10021	0.1000702	0.0001011
Н	2.6467877	-4.4611957	0.9217248
C	1 5000000	0 0770007	0 1505100
C	1.5809029	2.0110901	-0.1525130
F	-4 6424081	2 4530193	3 7176639
-	1.0121001	2.1000100	0.1110000
С	3.9850898	-1.5566177	0.0286479
ä		0.4440050	0.0408458
C	1.9499951	-2.4118356	0.3427457
C	0 1517569	0 0050001	0 197/030
C	-0.4517508	2.0252261	0.1074030
С	4 3260363	3 1414321	-0 2568455
	1.0200000	0.1111021	0.2000100
Н	4.5475365	4.1956411	-0.2251655
C	6 2441606	0 7076012	0 0003010
C	0.3441606	-0./8/6213	-0.0003819
C	-3 0603724	1 7358110	2 1304968
0	-5.0005124	1.7550115	2.1004000
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	0.0000704	4 4504000	
н	-2.6822731	-1.6534382	1.2681981
C	0 09/0590	0 /071227	0 1013300
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С	-1 3390443	0 9619864	0 4719807
	1.0000110	0.0010001	0.1110001
С	-3.7701720	1.2198317	-0.0760352
a	2 020000	0 5414060	0 0000740
C	3.0308988	2.5414260	-0.2890742
C	_0 7317037	-2 6208181	0 9485017
0	0.1011001	2.0200101	0.0100011
Н	-0.9105196	-3.6379471	1.2566474
a	4 5107400	0.0756540	0 0706706
C	4.519/498	0.8756549	-0.2/86/06
C	-4 3601207	2 0569066	2 4861187
0	-4.0001207	2.0000000	2.4001107
С	-5.0764567	1.5388748	0.2561809
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C	4.1421224	-2.925/182	0.4110948
U	E 0760910	2 1/07017	0 5200051
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С	-2.7385193	1.3123493	0.8482739
~	2.1.000100	1 5005050	
С	8.4145141	-1.5307950	-1.0140256
C	0 7004040	2 0775240	0 0002020
C	0.7094240	5.9115542	0.0603939
н	0 9781997	5 0208496	0 1065811
~	5.5.51001		
С	7.0635932	-1.2369127	-1.0990488
<u>~</u>	E 04740E0	0 1060265	0 0545020
C	5.2474052	2.1068365	-0.2545932
н	6 3206268	2 2128040	-0 2246618
11	0.0200200	2.2120040	-0.2240010
С	9.0708167	-1.3779764	0.1961931
~	7 0000444	0 0407574	4 4000070
C	7.0260411	-0.6427571	1.1998076
C	5 3700746	1 9583856	1 5/30705
0	-0.0100140	1.0002000	1.0402100
Dime	$r \text{ or } 1_{2}$		
	2		
N-	0 2671701	1 2075540	0 000000
TN T	0.30/1/31	1.32/3312	0.0000000
F	-1.1816182	0 9042232	5 3566523
-	1.1010102	0.0072202	0.0000020
F	2.4627793	3.6216580	4.0989818
F	0 7000404	1 1170700	6 6004004
L,	2.1222191	4.41/8/82	0.0234801
F	1.0344388	3,4969754	8.5335554
-	2.0011000		
F.	-0.9235566	1./421044	1.865/082
F	2 4627702	3 6216580	_4 0000010
1	2.1021130	0.0210000	-1.0303010
F	-1.1816182	0.9042232	-5.3566523
NT	1 6503100	1 0/0/7/4	1 0047100
TN	1.0023192	1.0424/41	1.204/193
Ν	1.6523192	1.0424741	-1.2047193
	1.0020102		1.2011100
C	0.5184426	1./588325	3.2053035

Ν	-0.8362037	1.8593789	-1.2122320
F	-0.9235566	1.7421044	-7.8657082
F	1.0344388	3.4969754	-8.5335554
С	1.7767657	3.5449386	6.3076398
N	-0 8362037	1 8593789	1 2122320
C	_1 9812439	2 3841373	_0 7163083
ĉ	2 0007220	0 9622021	2 067/600
	2.3301330	0.8032031	-2.90/4099
п	3.3000220	0.8002082	-3.9849843
C	-2.6944378	2.9406427	1.8395433
Н	-3.6547983	3.4297084	1.8089378
С	2.8595623	0.6690112	-0.7168114
F	2.7222191	4.4178782	-6.6234801
С	-0.6976105	2.0662059	2.5306242
С	-1.9812439	2.3841373	0.7163083
С	1.6551134	1.2211477	-2.5347617
С	3.7284738	0.5324131	1.8587791
н	4 7647464	0 2355982	1 8419980
C	0 6547020	0.2000002	1 6106//3
ĉ	1 6272522	2.1920030	F 0012401
å	1.03/3533	3.105/339	-5.0013491
0	-1.9151763	2.7522002	-2.945/138
Н	-2.1566814	3.061/02/	-3.9498/6/
С	-0.6976105	2.0662059	-2.5306242
С	0.5184426	1.7588325	-3.2053035
С	-0.2064107	1.7681669	-5.6270918
С	2.8595623	0.6690112	0.7168114
С	-2.6944378	2.9406427	-1.8395433
Н	-3.6547983	3.4297084	-1.8089378
С	1.6551134	1.2211477	2,5347617
Ċ	1 7767657	3 5449386	-6 3076398
ĉ	_0 0892127	2 1927388	-6 9388689
ĉ	1 0151762	2.1527000	0.0000000
U U	-1.3131703	2.1322002	2.9407130
п	-2.1500014	5.001/02/	3.9490101
C	0.6547029	2.1926036	-4.6196443
С	-0.0892127	2.1927388	6.9388689
С	3.7284738	0.5324131	-1.8587791
Н	4.7647464	0.2355982	-1.8419980
С	-0.2064107	1.7681669	5.6270918
С	2.9987338	0.8632031	2.9674699
Н	3.3555228	0.8662682	3.9849843
С	0.9114634	3.0840072	7.2840258
С	1.6373533	3.1057339	5.0013491
C	0.9114634	3.0840072	-7.2840258
Ni	_0 3671731	_1 3275512	0 0000000
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г Г	2 4627702	-0.9042232	-0.000020
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F	1.1816182	-0.9042232	5.3566523
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Ν	-1.6523192	-1.0424741	1.2047193
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c	-1 7767657	-3 5449386	-6 3076398
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C	2.6944378	-2.9406427	-1.8395433
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С	-2.8595623	-0.6690112	0.7168114
F	-2.7222191	-4.4178782	6.6234801
С	0.6976105	-2.0662059	-2.5306242
С	1.9812439	-2.3841373	-0.7163083
С	-1.6551134	-1.2211477	2.5347617
С	-3.7284738	-0.5324131	-1.8587791

Н	-4.7647464	-0.2355982	-1.8419980
С	-0.6547029	-2.1926036	-4.6196443
С	-1.6373533	-3.1057339	5.0013491
С	1.9151763	-2.7522002	2.9457138
Н	2.1566814	-3.0617027	3.9498767
С	0.6976105	-2.0662059	2.5306242
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	2.0944370	-2.9400427	1.0000070
H	3.654/983	-3.4297084	1.8089378
C	-1.6551134	-1.22114//	-2.534/61/
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С	0.0892127	-2.1927388	6.9388689
С	1.9151763	-2.7522002	-2.9457138
H	2.1566814	-3.0617027	-3.9498767
С	-0.6547029	-2.1926036	4.6196443
С	0.0892127	-2.1927388	-6.9388689
Ċ	-3 7284738	-0.5324131	1 8587791
н	_4 7647464	-0 2355982	1 8419980
C	0.206/107	1 7681660	5 6270018
d	0.2004107	-1.7001003	-0.0270910
	-2.998/338	-0.8632031	-2.96/4699
H	-3.3555228	-0.8662682	-3.9849843
С	-0.9114634	-3.0840072	-7.2840258
С	-1.6373533	-3.1057339	-5.0013491
С	-0.9114634	-3.0840072	7.2840258
Pheny	yl-substituted	dimer with C_2 sy	mmetry or 2_2
Ni	-1.1544643	-0.8711229	0.0120983
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н	-3 8620005	-0 2115500	4 5410863
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п 11	-4.3103707	-0.3202000	0.9070109
п 11	-2.044/0/0	-1.0904190	0.5177239
п	-0.3118299	-1.7066288	7.6293046
Н	-3.3889821	-0.9523312	-4.8456332
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Ν	-2.0580748	0.2226513	1.1160989
N	-1.9249232	0.0749982	-1.3005578
С	-1.5613038	-0.8331546	3.2510013
N	-0.4318307	-2.0852857	-1.1056461
Н	0.7221470	-2.0356188	-7.3540894
Н	-1.4020704	-1.6529137	-8.5728492
С	-3.3333048	-0.5934915	6.5797017
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C	0.0740989	-3.9303854	2.1193217
Н	0.4637254	-4.9342845	2.1604436
С	-2.5958965	1.1737241	-0.9241443
Н	-3.4616669	-1.1174139	-7.3014472
С	-0.8513993	-1.9028558	2.6703125
С	-0.0394944	-3.1063443	0.9413256
С	-1.8715468	-0.0867040	-2.6547428
С	-3.1278074	2.1156717	1.5869277
н	-3.6452992	3.0559348	1,4889699
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С	-1.2315139	-1.1994056	-3.2335260
С	-0.1439994	-1.7090055	-5.4265225
С	-2.6623870	1.2878929	0.5330763
С	0.3210378	-4.1356520	-1.5565512
Н	0.7188670	-5.1312710	-1.4447263
С	0 1000000	0 0051404	
	-2.1067259	0.2651424	2.4654540
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С	-0.4267636	-3.2034166	3.1728869
Н	-0.5150450	-3.5475969	4.1890401
С	-1.2886768	-1.3673247	-4.6967893
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C	-3.0284/16	1.8277124	-2.1302144
Н	-3.5789975	2.7510599	-2.1943955
С	-0.8403395	-1.3104985	5.5972242
С	-2.7842981	1.4856163	2.7879027
н	-2.9808305	1.8653743	3.7757094
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0 0	2.0441000		F 0104066
C ~	-3.0/8/698	-0.5194505	5.2184266
С	-1.3722535	-1.5811183	-7.4931830
Ni	1.1544643	0.8711229	0.0120983
Н	-0.7854324	1.8588925	-4.9011152
н	3.3889821	0.9523312	-4.8456332
 ц	3 1616669	1 117/130	7 301//72
11 TT	1 4000704	1.000127	-1.3014472
н	1.4020704	1.6529137	-8.5728492
Н	-0.7221470	2.0356188	-7.3540894
Н	3.8620005	0.2115500	4.5410863
Н	-0.1457191	1.5440709	5.2249419
N	1,9249232	-0.0749982	-1.3005578
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N N	2.0000740	-0.2220013	1.1100909
C	1.2315139	1.1994056	-3.2335260
Ν	0.5569384	1.9332892	1.3345267
Н	0.3118299	1.7066288	7.6293046
Н	2.5447573	1.0904190	8.5177239
С	2 5247596	1 2704807	-6 7808812
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N	0.4316307	2.0052057	-1.1050401
С	0.0394944	3.1063443	0.9413256
С	2.7842981	-1.4856163	2.7879027
Н	2.9808305	-1.8653743	3.7757094
С	-0.3210378	4.1356520	-1.5565512
н	-0 7188670	5 1312710	-1 4447263
Ċ	0.1100010	1 2070020	0 5220762
	2.0023070	-1.2070929	0.000000
н	4.3105/8/	0.3202600	6.95/3109
С	0.5628137	2.2205079	-2.4426864
С	-0.0637760	3.2027685	-0.5142559
С	2.1067259	-0.2651424	2.4654540
Ċ	3 0284716	-1 8277124	-2 1302144
ц ц	3 5780075	2 7510500	2 10/3055
n a	3.0109910	-2.7510599	-2.1943933
C	1.2886/68	1.36/324/	-4.696/893
С	3.0787698	0.5194505	5.2184266
С	0.4267636	3.2034166	3.1728869
Н	0.5150450	3.5475969	4.1890401
С	0 8513993	1 9028558	2 6703125
c	1 5612020	0.9331546	2.0100120
0	1.0010000	0.0331340	5.2510013
C	0.8403395	1.3104985	5.5972242
С	2.5958965	-1.1737241	-0.9241443
С	-0.0740989	3.9303854	2.1193217
Н	-0.4637254	4.9342845	2.1604436
С	1.8715468	0.0867040	-2.6547428
c	2 2222040	0 503/015	6 5707017
0	1 0070007	1 2002054	0.5797017
C ~	1.0976997	1.3883954	6.9570048
С	0.0670552	3.5320281	-2.7530340
Н	0.0174576	3.9787572	-3.7318476
С	1.8262151	0.8793209	4.6994009
Ċ	0 1832012	1 8047825	-6 8082639
c	2 1072074	0 1156717	1 5960077
	3.12/00/4	-2.1150717	1.0009277
п	3.0452992	-3.0559348	1.4889699
С	0.1439994	1.7090055	-5.4265225
С	2.5847683	-1.0651820	-3.1882718
Н	2.7452805	-1.2810848	-4.2299319
С	1.3722535	1.5811183	-7,4931830
ĉ	2 101 22000 2 101/72F	1 1656001	_5 2077027
ä	2.7044100	1.1000091	-0.0311901
C	2.3441086	1.0299108	1.4558/8/
		a .	
Mono	mer without p	pentafluoropheny	/l groups or $1'$
Ni	-0.0000123	0.1036975	0.4184611
Ν	1.2122121	-1.2067988	0.6247207

Ν	-1.2107946	-1.2077371	0.6229743
С	3.2095997	0.0209327	0.0763054
Ν	-1.2136114	1.3669273	0.0158621
Ν	1.2122592	1.3679287	0.0160783
С	-0.7512069	2.5222135	-0.4445187
С	-2.9884140	-2.5452624	0.5363164
Η	-4.0031189	-2.9025952	0.4547349
С	1.8587756	3.2841440	-0.9027320
Н	1.8316842	4.2734194	-1.3294367
С	-0.7491842	-2.4430251	0.7636275
С	2.5606700	1.2573244	-0.1475031
С	0.7489857	2.5228239	-0.4441149
С	-2.5614179	-1.1834855	0.4416548
С	1.8650089	-3.3267762	0.7308534
Η	1.8409206	-4.4001479	0.8242123
Н	4.2759265	-0.0237584	-0.1102484
С	-2.9870337	2.4962534	-0.7174450
Н	-3.9997956	2.7672006	-0.9722278
С	-2.5617869	1.2551151	-0.1483655
С	-3.2100415	0.0181925	0.0755881
С	0.7514115	-2.4426263	0.7640517
С	-1.8613494	3.2821525	-0.9042197
Н	-1.8349685	4.2711662	-1.3315798
С	2.5625090	-1.1814863	0.4428000
С	2.9850496	2.4993653	-0.7154804
Н	3.9977491	2.7716198	-0.9690587
Η	-4.2763717	-0.0275471	-0.1105462
С	-1.8622803	-3.3278548	0.7317922
Η	-1.8375561	-4.4011239	0.8262165
С	2.9906192	-2.5431050	0.5354676
Н	4.0055770	-2.8994776	0.4530703

Dimer without pentafluorophenyl groups or $\mathbf{1}_2'$

Ni	-1.3631938	-0.1972603	0.000000
Ν	-1.6185891	1.0941124	1.2047196
Ν	-1.6185891	1.0941124	-1.2047196
С	-1.8189081	-0.2320544	3.2053042
Ν	-1.3666084	-1.5129143	-1.2122323
Ν	-1.3666084	-1.5129143	1.2122323
С	-1.3869924	-2.7723084	-0.7163085
С	-1.9954924	2.3990703	-2.9674705
Н	-2.1416763	2.7245516	-3.9849851
С	-1.6099866	-3.6490169	1.8395437
Н	-1.6719010	-4.7249559	1.8089382
С	-1.7617434	2.3496673	-0.7168116
С	-1.6116950	-1.4691183	2.5306247
С	-1.3869924	-2.7723084	0.7163085
С	-1.7833240	1.0248703	-2.5347622
С	-1.9858358	3.2002254	1.8587795
Η	-2.1304718	4.2684206	1.8419984
Н	-2.0207841	-0.2483307	4.2667731
С	-1.7505786	-2.8597177	-2.9457144
Н	-1.9369414	-3.2052398	-3.9498775
С	-1.6116950	-1.4691183	-2.5306247
С	-1.8189081	-0.2320544	-3.2053042
С	-1.7617434	2.3496673	0.7168116
С	-1.6099866	-3.6490169	-1.8395437
Η	-1.6719010	-4.7249559	-1.8089382
С	-1.7833240	1.0248703	2.5347622
С	-1.7505786	-2.8597177	2.9457144
Н	-1.9369414	-3.2052398	3.9498775
Η	-2.0207841	-0.2483307	-4.2667731
С	-1.9858358	3.2002254	-1.8587795
Н	-2.1304718	4.2684206	-1.8419984
С	-1.9954924	2.3990703	2.9674705
Η	-2.1416763	2.7245516	3.9849851
Ni	1.3631938	0.1972603	0.000000
N	1.6185891	-1.0941124	-1.2047196
Ν	1.6185891	-1.0941124	1.2047196

C	1.8189081	0.2320544	-3.2053042
Ν	1.3666084	1.5129143	1.2122323
Ν	1.3666084	1.5129143	-1.2122323
С	1.3869924	2.7723084	0.7163085
С	1,9954924	-2.3990703	2,9674705
й	2 1/16763	2.22000100	3 08/0851
2	1 6000866	2.72400160	1 0205427
C	1.6099866	3.6490169	-1.8395437
Н	1.6719010	4.7249559	-1.8089382
С	1.7617434	-2.3496673	0.7168116
С	1.6116950	1.4691183	-2.5306247
С	1.3869924	2.7723084	-0.7163085
Ĉ	1 78330/0	1 02/8703	2 5347622
å	1.7055240	-1.0240703	1 0507705
C	1.9858358	-3.2002254	-1.858//95
Н	2.1304718	-4.2684206	-1.8419984
Н	2.0207841	0.2483307	-4.2667731
С	1.7505786	2.8597177	2.9457144
н	1 9369414	3 2052398	3 9498775
ĉ	1 6116050	1 4601193	2 5206247
å	1.0110950	1.4091103	2.0300247
C	1.8189081	0.2320544	3.2053042
С	1.7617434	-2.3496673	-0.7168116
С	1.6099866	3.6490169	1.8395437
Н	1.6719010	4.7249559	1.8089382
C	1 7833240	_1 0248703	-2 5347622
ĉ	1 7605796	0 0507177	2.0047022
C	1.7505786	2.859/1//	-2.945/144
Н	1.9369414	3.2052398	-3.9498775
Н	2.0207841	0.2483307	4.2667731
С	1.9858358	-3.2002254	1.8587795
н	2 1304718	-4.2684206	1 8419984
ĉ	1 005/02/	2 3000703	2 967/705
	1.9904924	-2.3990703	-2.9014105
н	2.1416/63	-2.7245516	-3.9849851
Ero	o baco porcorrol		
гıе	e-Dase norcorror	5	
Ν	1.7144615	-0.0132479	-0.0000178
N C	1.7144615 2.2597758	-0.0132479 -1.2077326	-0.0000178 -0.0000305
N C C	1.7144615 2.2597758 2.6914494	-0.0132479 -1.2077326 0.9646455	-0.0000178 -0.0000305
N C C	1.7144615 2.2597758 2.6914494	-0.0132479 -1.2077326 0.9646455	-0.0000178 -0.0000305 -0.0000198
N C C C	1.7144615 2.2597758 2.6914494 3.7052271	-0.0132479 -1.2077326 0.9646455 -1.0725094	-0.0000178 -0.0000305 -0.0000198 -0.0000410
N C C C C	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725	-0.0000178 -0.0000305 -0.0000198 -0.0000410 -0.0000237
N C C C H	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306	-0.0000178 -0.0000305 -0.0000198 -0.0000410 -0.0000237 -0.0000680
N C C C H H	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082 4.9447287	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625	-0.0000178 -0.0000305 -0.0000198 -0.0000410 -0.0000237 -0.0000680 -0.000098
N C C C H H N	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082 4.9447287 0.0038355	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918	-0.000178 -0.000305 -0.000198 -0.0000410 -0.0000237 -0.0000680 -0.000098 0.0000054
N C C C H H N	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082 4.9447287 0.0038355 0.2820471	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 0.929097	-0.000178 -0.0000305 -0.0000198 -0.0000410 -0.0000237 -0.0000680 -0.0000098 0.0000054
N C C C H H N H	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082 4.9447287 0.0038355 -0.2829471	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987	-0.000178 -0.000305 -0.000198 -0.0000410 -0.0000237 -0.0000680 -0.000098 0.000054 0.0000197
N C C H H N H N	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479	-0.000178 -0.0000305 -0.0000198 -0.0000410 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 0.0000119
N C C C H H N H N N	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918	-0.0000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000054 0.0000054 0.0000197 0.0000119 -0.0000001
N C C C H H N H N H	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987	-0.0000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 0.0000119 -0.0000001 -0.0000202
N C C C C H H N H N H C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511	-0.000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 -0.00000119 -0.0000001 -0.0000202 0.0000195
N C C C C H H N H N H C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326	-0.0000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 0.0000119 -0.0000001 -0.00000202 0.0000195 -0.00000095
N C C C C H H N H N N H C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.0550262\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000680 -0.0000054 0.0000197 0.0000119 -0.000001 -0.0000202 0.0000195 -0.0000009
N C C C C H H N H N N H C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000080 -0.0000098 0.0000197 0.0000119 -0.000001 -0.000001 -0.0000202 0.0000195 -0.000009 0.0000110
N C C C C H H N H N N H C C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280	$\begin{array}{c} -0.0000178\\ -0.0000305\\ -0.0000198\\ -0.0000237\\ -0.0000237\\ -0.0000058\\ 0.0000054\\ 0.0000197\\ 0.0000119\\ -0.0000001\\ -0.0000202\\ 0.0000195\\ -0.000009\\ 0.0000110\\ -0.0000110\\ -0.0000180\end{array}$
N C C C C H H N H N N H C C C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455	-0.000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000054 0.0000197 -0.00000119 -0.0000001 -0.0000202 0.000109 -0.000009 0.000010 -0.000010 -0.0000180 0.0000130
И С С С С Н Н И Н И И Н С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000680 -0.0000054 0.0000197 0.0000197 -0.00000197 -0.0000001 -0.0000009 0.0000195 -0.0000180 0.000043 0.0000178
И С С С С Н Н И Н И И Н С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -3.9976949	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000680 -0.000098 0.000054 0.0000197 0.0000119 -0.00000119 -0.0000202 0.0000195 -0.0000010 -0.0000118 0.0000178
И С С С С Н Н И Н И И Н С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ 3.7052271\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000098 0.000054 0.0000197 0.0000197 -0.000001 -0.0000202 0.0000195 -0.0000010 -0.0000110 -0.0000180 0.0000178 0.0000026 0.0000166
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ -0.965045\\ -3.7052271\\ -3.705227$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 2.276240	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000098 0.000054 0.0000197 0.0000197 -0.000001 -0.0000202 0.000195 -0.000009 0.0000110 -0.0000180 0.0000178 0.000026 -0.0000166
N C C C C H H N H N N H C C C C C C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949	$\begin{array}{c} -0.0000178\\ -0.0000305\\ -0.0000198\\ -0.0000237\\ -0.0000680\\ -0.000098\\ 0.0000054\\ 0.0000197\\ -0.00000119\\ -0.00000119\\ -0.0000001\\ -0.00000202\\ 0.0000195\\ -0.0000009\\ 0.0000110\\ -0.0000180\\ 0.0000178\\ 0.0000178\\ 0.0000178\\ 0.000026\\ -0.0000166\\ 0.0000357\end{array}$
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195	$\begin{array}{c} -0.0000178\\ -0.0000305\\ -0.0000198\\ -0.0000237\\ -0.0000237\\ -0.0000680\\ -0.000098\\ 0.0000054\\ 0.0000197\\ 0.0000119\\ -0.00000119\\ -0.0000001\\ -0.0000195\\ -0.0000195\\ -0.0000110\\ -0.0000180\\ 0.0000118\\ 0.0000178\\ 0.0000178\\ 0.0000178\\ 0.000026\\ -0.0000166\\ 0.0000357\\ 0.0000501\end{array}$
N C C C C H H N H N N H C C C C C C C C	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725	-0.000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 0.0000119 -0.0000001 -0.0000001 0.0000105 -0.00000180 0.0000178 0.0000043 0.0000178 0.0000166 0.0000357 0.0000501 -0.0000314
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000680 -0.000098 0.0000197 0.0000197 -0.0000119 -0.0000101 -0.0000195 -0.0000110 -0.0000180 0.0000178 0.0000178 0.0000166 0.0000357 0.0000501 -0.0000314
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 -0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195 -4.9826235	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.000098 0.000054 0.0000197 0.0000197 -0.000001 -0.0000202 0.0000195 -0.0000100 -0.0000110 -0.0000180 0.0000180 0.0000178 0.0000166 0.0000357 0.0000314 0.0000181 -0.0000181
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ 4.4271022\\ \end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195 -4.9826235 1.8727202	-0.000178 -0.0000305 -0.0000198 -0.0000237 -0.0000680 -0.0000098 0.0000054 0.0000197 -0.0000019 -0.0000001 -0.0000202 0.000110 -0.0000109 0.0000110 -0.0000180 0.0000178 0.0000178 0.0000178 0.0000178 0.0000166 0.0000357 0.0000501 -0.0000314 0.0000619 0.00000619
И С С С С Н Н И Н И И Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -0.7033329\\ -4.4271082\\ -0.7033329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -4.4271082\\ -0.703329\\ -0.70329\\ -0.70329\\ -0.70329\\ -0.70329\\ -0.70329\\$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195 -4.9826235 1.8737306	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000680 -0.000098 0.000054 0.0000197 -0.0000197 -0.00000197 -0.00000195 -0.0000195 -0.0000100 -0.0000180 0.0000180 0.0000178 0.0000178 0.0000178 0.0000178 0.0000166 -0.0000166 0.0000357 0.0000501 -0.0000314 0.0000181 -0.0000199 -0.000099
И С С С С Н Н И Н И И И С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.703329\end{array}$	$\begin{array}{c} -0.0132479\\ -1.2077326\\ 0.9646455\\ -1.0725094\\ 0.2766725\\ -1.8737306\\ 0.7404625\\ -1.8187918\\ -0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ -2.7659511\\ 1.2077326\\ 2.7659511\\ -2.2997280\\ -0.9646455\\ 2.2997280\\ -3.9976949\\ 1.0725094\\ 3.9976949\\ 1.0725094\\ 3.9976949\\ -3.7048195\\ -0.2766725\\ 3.7048195\\ -4.9826235\\ 1.8737306\\ 4.9826235\\ \end{array}$	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000680 -0.000098 0.0000197 0.0000197 -0.0000197 -0.00000197 -0.00000195 -0.0000109 -0.0000110 -0.0000110 -0.0000180 0.0000178 0.0000178 0.0000178 -0.0000166 -0.0000166 -0.0000181 -0.0000181 -0.0000699 -0.0000692
И С С С С Н Н И И И И И С С С С С С С С	1.7144615 2.2597758 2.6914494 3.7052271 3.9701805 4.4271082 4.9447287 0.0038355 -0.2829471 -1.7144615 -0.0038355 0.2829470 -0.9650363 -2.2597758 0.9650363 1.2532163 -2.6914494 -1.2532163 -0.2650645 -3.7052271 0.2650645 1.1165422 -3.9701805 -1.1165422 -0.703329 -4.4271082 0.703329 1.9166348	$\begin{array}{c} -0.0132479\\ -1.2077326\\ 0.9646455\\ -1.0725094\\ 0.2766725\\ -1.8737306\\ 0.7404625\\ -1.8187918\\ -0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ -2.7659511\\ 1.2077326\\ 2.7659511\\ -2.2997280\\ -0.9646455\\ 2.2997280\\ -3.9976949\\ 1.0725094\\ 3.9976949\\ 1.0725094\\ 3.9976949\\ -3.7048195\\ -0.2766725\\ 3.7048195\\ -4.9826235\\ 1.8737306\\ 4.9826235\\ -4.4262251\\ \end{array}$	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.000098 0.000054 0.0000197 0.0000197 -0.00000197 -0.0000001 -0.0000109 -0.0000110 -0.0000178 0.0000178 0.0000178 0.0000178 0.0000178 -0.0000166 0.0000357 0.0000501 -0.0000314 0.0000181 -0.0000692 0.0000692 0.0001568
И С С С С Н Н И И И И И С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.703329\\ 1.9166348\\ -4.9447287\end{array}$	$\begin{array}{c} -0.0132479\\ -1.2077326\\ 0.9646455\\ -1.0725094\\ 0.2766725\\ -1.8737306\\ 0.7404625\\ -1.8187918\\ -0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ -2.7659511\\ 1.2077326\\ 2.7659511\\ -2.2997280\\ -0.9646455\\ 2.2997280\\ -3.9976949\\ 1.0725094\\ 3.9976949\\ 1.0725094\\ 3.9976949\\ -3.7048195\\ -0.2766725\\ 3.7048195\\ -0.2766725\\ 3.7048195\\ -4.9826235\\ 1.8737306\\ 4.9826235\\ -4.4262251\\ -0.7404625\end{array}$	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.000098 0.000054 0.0000197 0.0000197 -0.0000197 -0.0000195 -0.00000180 0.0000180 0.0000180 0.0000178 0.0000178 0.0000026 -0.0000166 0.0000357 0.0000501 -0.0000314 0.0000181 -0.0000199 -0.0000692 0.0001568 -0.0000726
N С С С С Н Н N Н N N Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.703329\\ 1.9166348\\ -4.9447287\\ -1.9166348\\ \end{array}$	$\begin{array}{c} -0.0132479\\ -1.2077326\\ 0.9646455\\ -1.0725094\\ 0.2766725\\ -1.8737306\\ 0.7404625\\ -1.8187918\\ -0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ -2.7659511\\ 1.2077326\\ 2.7659511\\ -2.2997280\\ -0.9646455\\ 2.2997280\\ -3.9976949\\ 1.0725094\\ 3.9976949\\ 1.0725094\\ 3.9976949\\ -3.7048195\\ -0.2766725\\ 3.7048195\\ -4.9826235\\ 1.8737306\\ 4.9826235\\ -4.4262251\\ -0.7404625\\ 4.4262251\\ \end{array}$	-0.000178 -0.000305 -0.000198 -0.000237 -0.0000237 -0.000098 0.0000054 0.0000197 -0.0000197 -0.0000197 -0.00000197 -0.00000202 0.000110 -0.0000109 0.0000110 -0.0000110 -0.0000180 0.0000178 0.0000178 0.0000178 0.0000166 0.0000357 0.0000501 -0.0000314 0.0000181 -0.0000199 0.0000692 0.0001568 -0.000726 -0.000006
N С С С С Н Н N Н N N Н С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -0.7033329\\ -4.4271082\\ 0.7033329\\ -4.4271082\\ 0.7033329\\ 1.9166348\\ -4.9447287\\ -1.9166348\\ -2.3278689\end{array}$	$\begin{array}{c} -0.0132479\\ -1.2077326\\ 0.9646455\\ -1.0725094\\ 0.2766725\\ -1.8737306\\ 0.7404625\\ -1.8187918\\ -0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ 0.0132479\\ 1.8187918\\ 0.8389987\\ -2.7659511\\ 1.2077326\\ 2.7659511\\ -2.2997280\\ -0.9646455\\ 2.2997280\\ -0.9646455\\ 2.2997280\\ -3.9976949\\ 1.0725094\\ 3.9976949\\ 1.0725094\\ 3.9976949\\ -3.7048195\\ -0.2766725\\ 3.7048195\\ -4.9826235\\ 1.8737306\\ 4.9826235\\ -4.4262251\\ -0.7404625\\ -4.4262251\\ -0.7404625\\ -4.4262251\\ -2.3078129\\ \end{array}$	-0.000178 -0.000305 -0.000198 -0.000237 -0.0000880 -0.000098 0.000054 0.0000197 -0.0000197 -0.0000197 -0.00000197 -0.00000195 -0.0000010 -0.0000100 -0.0000100 -0.0000180 0.0000178 0.0000178 0.0000166 0.0000501 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000183 -0.00001568 -0.0000726 -0.00000692 0.0001568 -0.0000726 -0.0000064
И С С С С Н Н И И И И И С С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.7033329\\ 1.9166348\\ -4.9447287\\ -1.9166348\\ -4.9447287\\ -1.9166348\\ -2.3278689\\ 2.3278689\\ -2.327869\\ -2.3278689\\ -2.32$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195 -4.9826235 1.8737306 4.9826235 -4.4262251 -0.7404625 4.4262251 -0.7404625 4.4262251 -2.3078129 2.3078129	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000680 -0.000098 0.0000197 0.0000197 -0.0000197 -0.00000197 -0.00000195 -0.0000099 0.0000110 -0.0000180 0.0000180 -0.0000180 -0.0000180 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000181 -0.0000183 -0.00001568 -0.0000726 -0.00000692 -0.0000064
И С С С С Н Н И И И И И И С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.703329\\ 1.9166348\\ -4.9447287\\ -1.9166348\\ -2.3278689\\ 2.3278689\\$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 1.2097280 -0.9646455 2.2997280 -3.9976949 1.0725094 3.9976949 1.0725094 3.9976949 -0.2766725 3.7048195 -0.2766725 3.7048195 -4.9826235 1.8737306 4.9826235 -4.4262251 -0.7404625 4.4262251 -2.3078129 2.3078129 2.3078129 2.3078129	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.0000680 -0.000098 0.0000197 0.0000197 -0.00000197 -0.00000195 -0.0000010 -0.0000100 -0.0000110 -0.0000110 -0.0000118 0.0000178 0.0000178 -0.0000166 0.0000166 -0.0000166 -0.0000166 -0.00001568 -0.00001568 -0.00001568 -0.0000164 -0.0000164 -0.0000164 -0.0000164 -0.0000164
И С С С С Н Н И И И И И И С С С С С С С	$\begin{array}{c} 1.7144615\\ 2.2597758\\ 2.6914494\\ 3.7052271\\ 3.9701805\\ 4.4271082\\ 4.9447287\\ 0.0038355\\ -0.2829471\\ -1.7144615\\ -0.0038355\\ 0.2829470\\ -0.9650363\\ -2.2597758\\ 0.9650363\\ 1.2532163\\ -2.6914494\\ -1.2532163\\ -0.2650645\\ -3.7052271\\ 0.2650645\\ 1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -3.9701805\\ -1.1165422\\ -0.703329\\ -4.4271082\\ 0.703329\\ 1.9166348\\ -4.9447287\\ -1.9166348\\ -2.3278689\\ 2.3278689\\ -3.1120492\end{array}$	-0.0132479 -1.2077326 0.9646455 -1.0725094 0.2766725 -1.8737306 0.7404625 -1.8187918 -0.8389987 0.0132479 1.8187918 0.8389987 -2.7659511 1.2077326 2.7659511 -2.2997280 -3.9976949 1.0725094 3.9976949 1.0725094 3.9976949 -3.7048195 -0.2766725 3.7048195 -4.9826235 1.8737306 4.9826235 -4.4262251 -0.7404625 4.4262251 -2.3078129 2.3078129 -3.0549562	-0.000178 -0.000305 -0.000198 -0.0000237 -0.0000237 -0.000098 0.000054 0.0000197 0.0000197 -0.00000197 -0.0000001 -0.0000109 -0.0000100 -0.0000180 0.0000178 0.0000178 0.0000178 0.0000178 0.0000178 -0.0000166 0.0000357 0.0000501 -0.0000501 -0.00001568 -0.00001568 -0.00001568 -0.0000164 -0.0000164 -0.000064 0.0000264