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ELECTRONIC SUPPLEMENTARY INFORMATION

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

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S1 Molecular orbitals

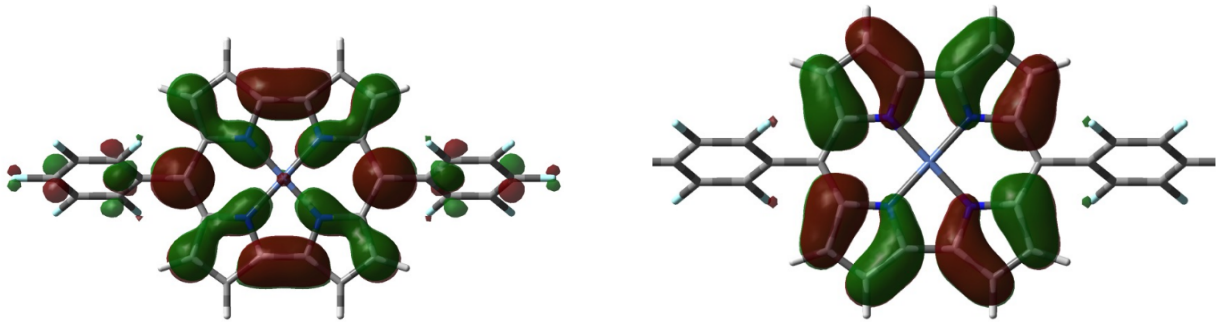

Fig. S1 The LUMO of the monomer (left) and the HOMO of the monomer (right)

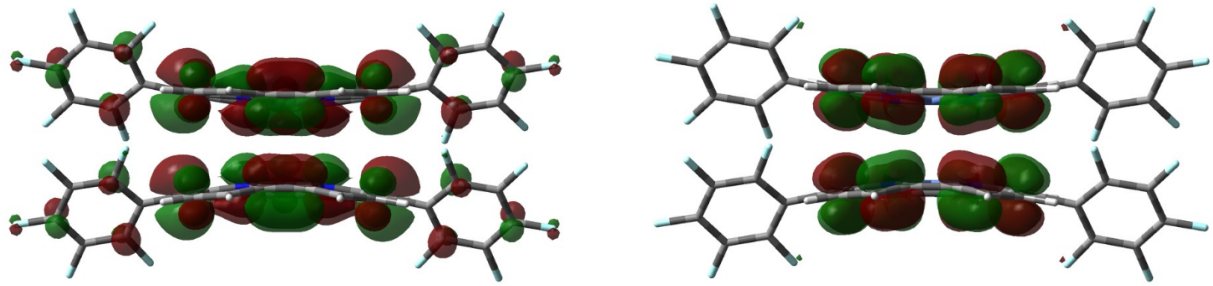

Fig. S2 The LUMO+1 of the dimer (left) and the LUMO of the dimer (right)

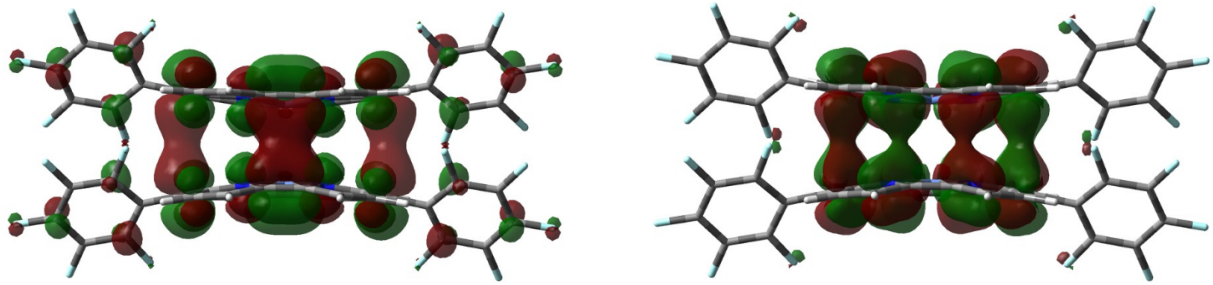

Fig. S3 The HOMO of the dimer (left) and the HOMO-1 of the dimer (right)

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

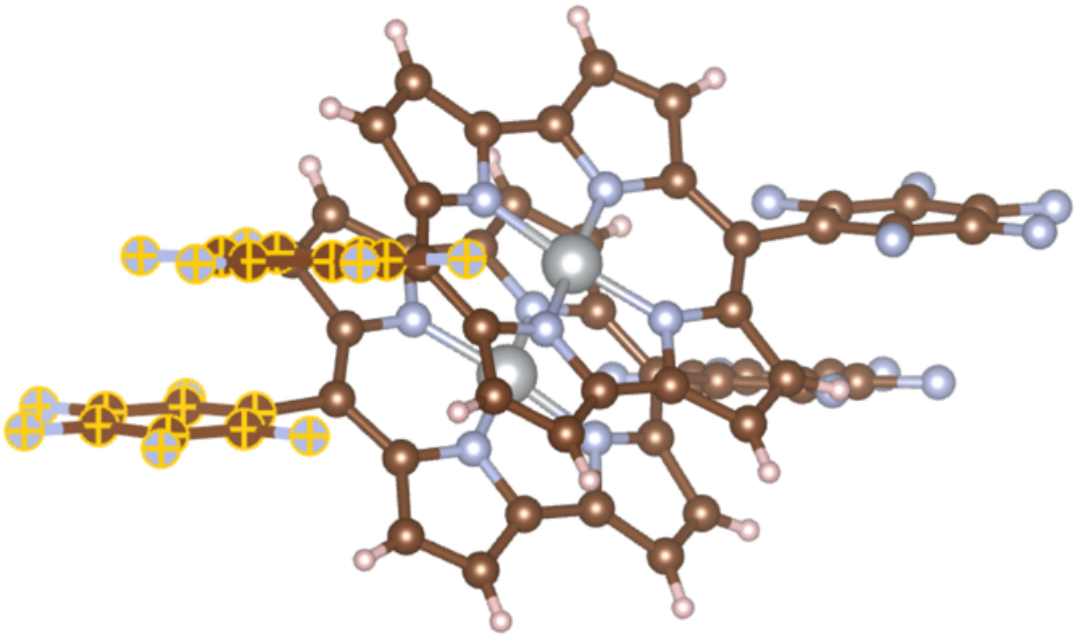

Fig. S4 The molecular structure of $\mathbf{1}_2$ seen from the side, which reveals the parallel orientation of the pentafluorophenyl substituents. The brown atoms are carbon, the blue ones are nitrogen, the nickel atoms are grey, and the hydrogen are pink. Two of the pentafluorophenyl substituents are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

S3 Current-density analysis

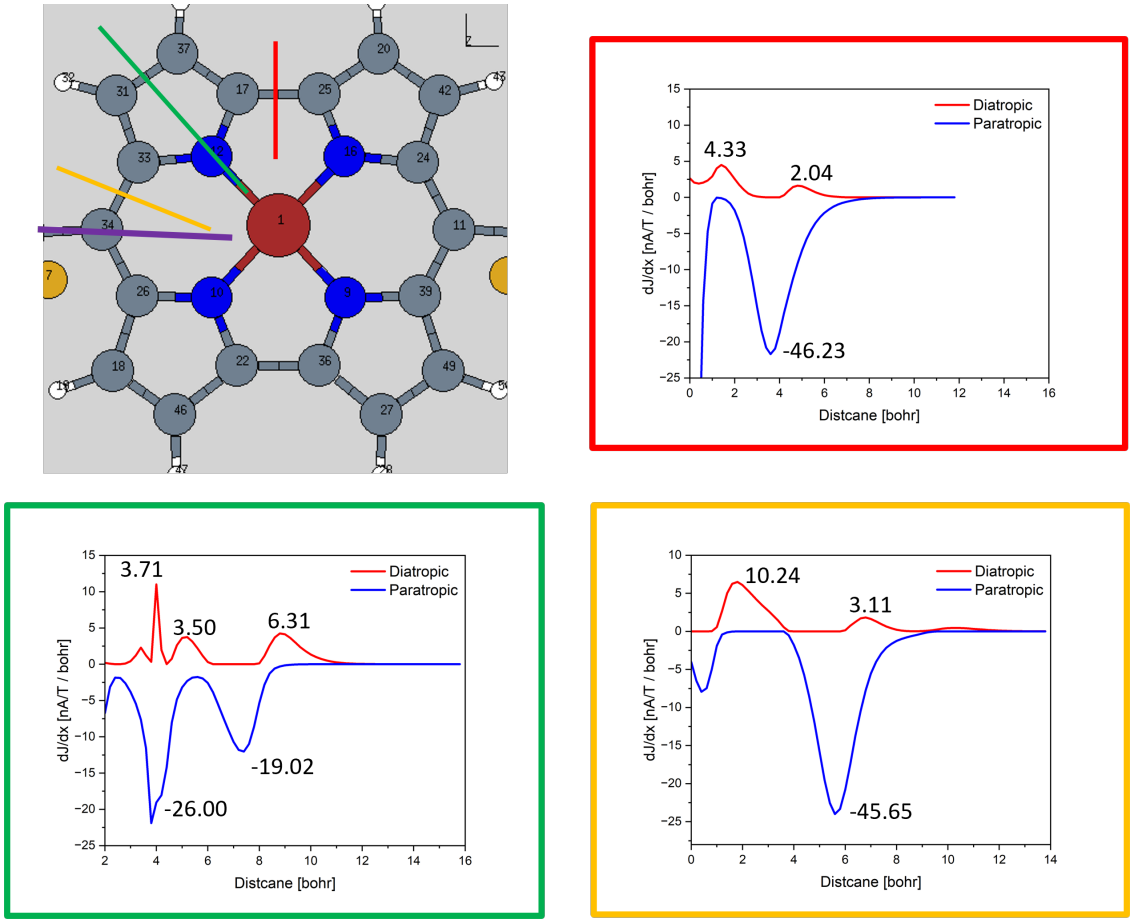

Fig. S5 The positions of the integration planes of **1** for determining the strength of the current-density pathways are shown with the colored lines in the upper-left picture. The current density is calculated at the CAM-B3LYP/def2-TZVP level. The three other pictures show the calculated ring-current 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.

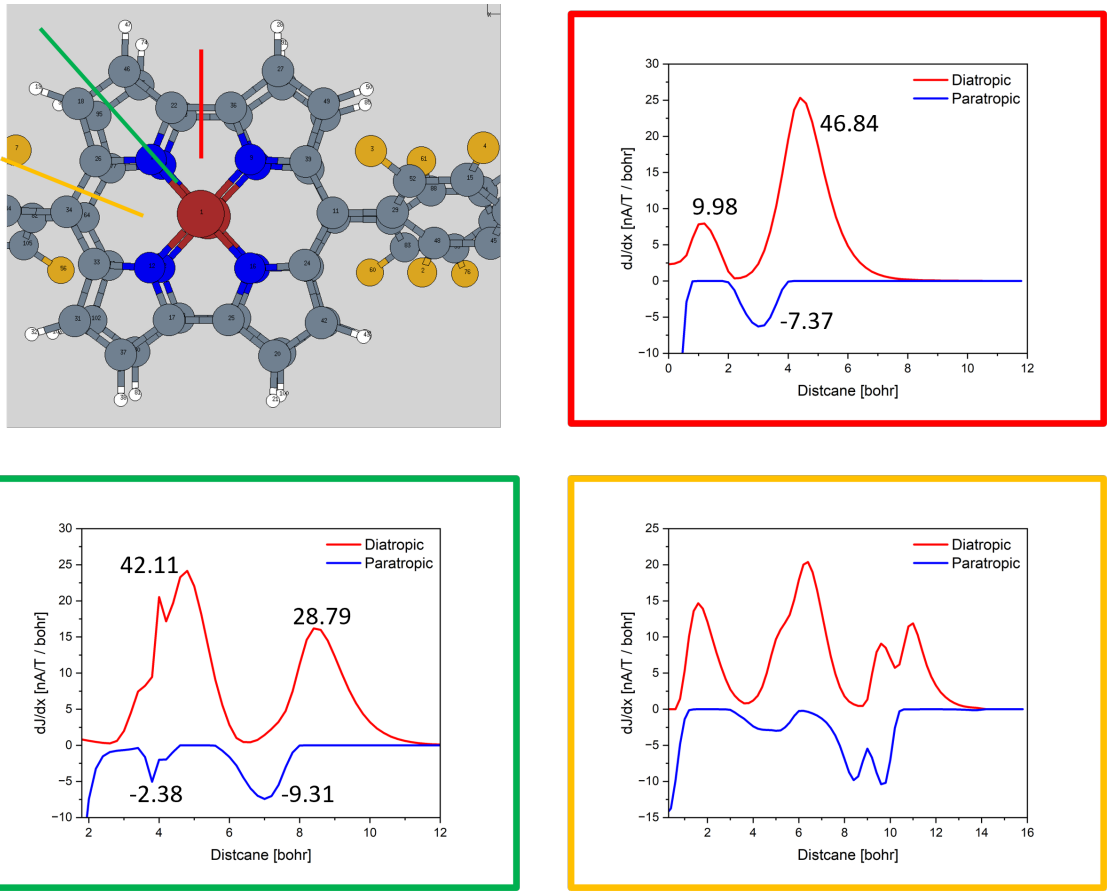

Fig. S6 The positions of the integration planes of $\mathbf{1}_2$ for determining the strength of the current-density pathways are shown with the colored lines in the upper-left picture. The current density is calculated at the CAM-B3LYP/def2-TZVP level. The three other pictures show the calculated ring-current 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.

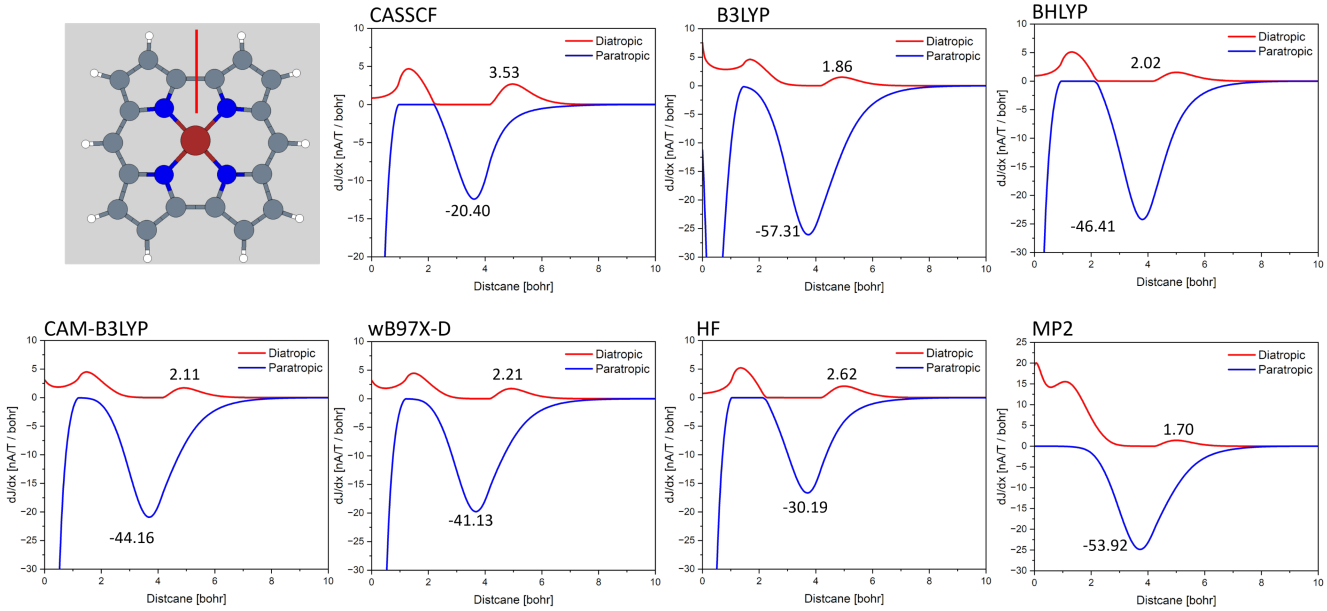

Fig. S7 The ring-current profile of $\mathbf{1}'$ passing through the red plane. The current density is calculated at different levels of theory. The pentafluorophenyl substituents are replace with hydrogen atoms.

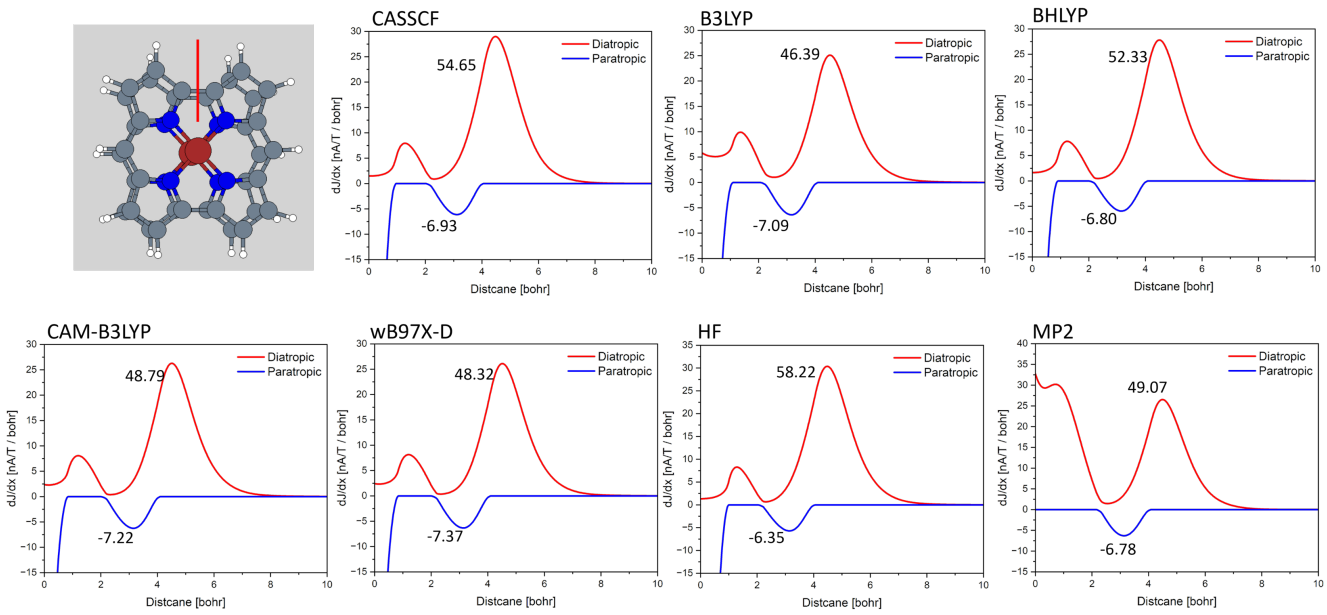

Fig. S8 The ring-current profile of $\mathbf{1}_2'$ passing through the red plane. The current density is calculated at different levels of theory. The pentafluorophenyl substituents are replace with hydrogen atoms.

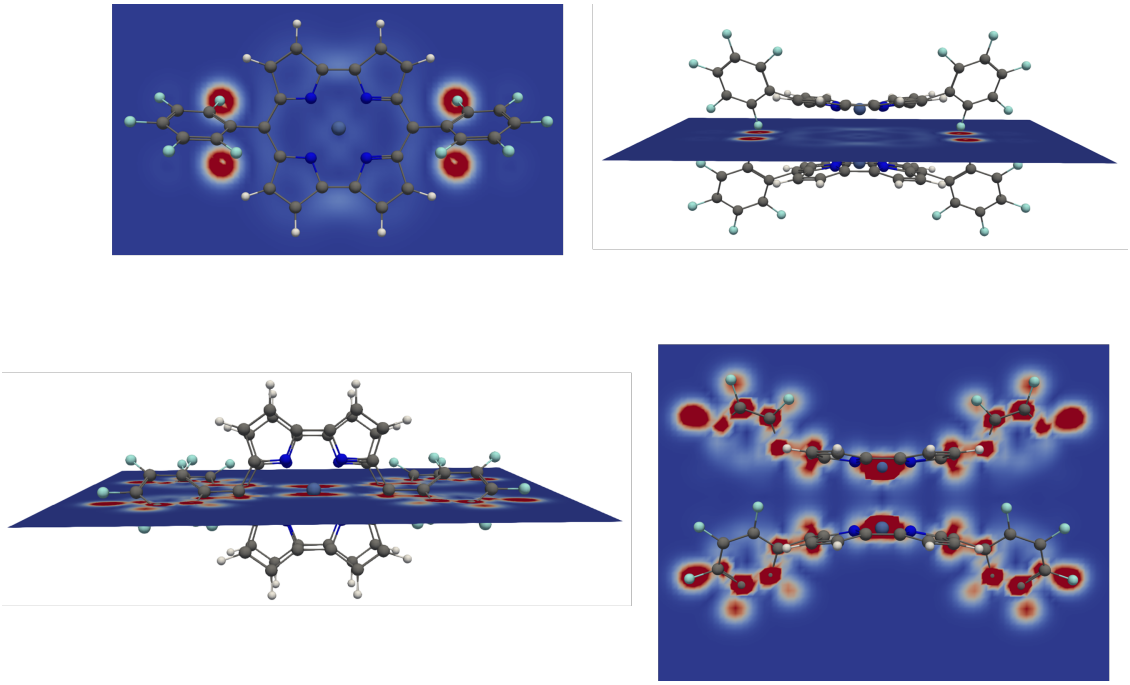

Fig. S9 The upper left picture is the top view of the current density crossing the plane which is perpendicular the external magnetic field as shown in the upper right picture. The four strong red spots are due to the adjacent H atoms. The lower right picture shows the current density passing a plane in the middle of $\mathbf{1}_2$. 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

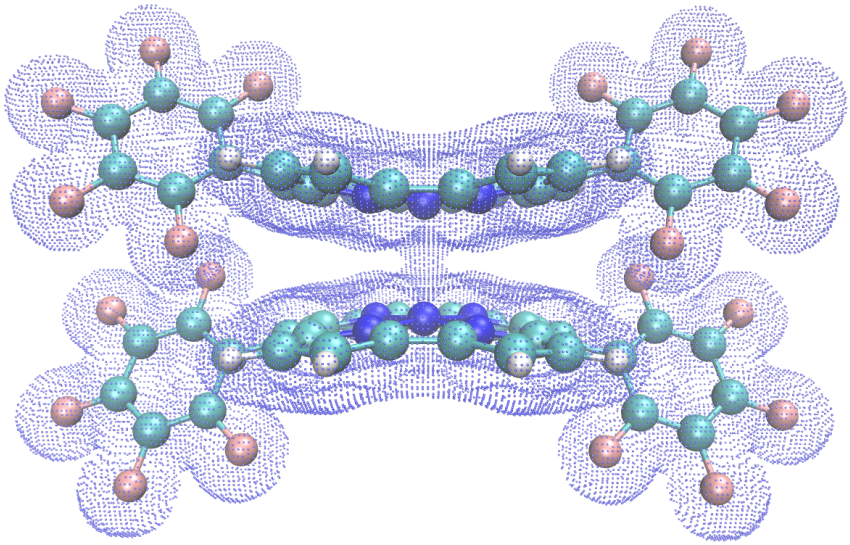

Fig. S10 The electron density of $\mathbf{1}_2$. The electron density between the two Ni atoms is seen.

S5 Isotropic nuclear magnetic shielding constants

S5.1 Monomer

Monomer 1H NMR shielding constants in beta position

Level	Average	H19	H21	H28	H32
B3LYP/TZVP	30.974303	30.858047	31.069241	31.097967	30.865421
BHLYP/TZVP	29.844912	29.654736	30.008080	30.029742	29.679327
CAM-B3LYP/TZVP	29.351458	29.178386	29.500103	29.516093	29.203741
wB97X-D/TZVP	29.002611	28.819628	29.161281	29.175052	28.846870
HF/TZVP	28.274654	27.921137	28.594187	28.602199	27.972123
HF/SVP	28.337066	28.066465	28.579962	28.580048	28.112918
MP2/SVP	31.112409	31.246931	30.978735	31.000035	31.220486

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

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

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

Level	Average	C20	C27	C37	C46
B3LYP/TZVP	66.031905	65.938668	66.118262	65.945586	66.125102
BHLYP/TZVP	69.273729	69.206393	69.334067	69.212684	69.341773
CAM-B3LYP/TZVP	67.224395	67.170318	67.270423	67.181597	67.275243
wB97X-D/TZVP	69.645828	69.598012	69.685051	69.609716	69.690533
HF/TZVP	78.004785	77.991878	78.011017	78.003501	78.012744
HF/SVP	88.747752	88.735640	88.747041	88.750418	88.757909
MP2/SVP	93.762020	93.616816	93.898151	93.607028	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	48.175593	48.261886	48.057676	48.064162	48.318649
BHLYP/TZVP	46.218602	46.250518	46.157665	46.141392	46.324831
CAM-B3LYP/TZVP	46.042281	46.074708	45.979860	45.966890	46.147667
wB97X-D/TZVP	49.006877	49.031052	48.951925	48.940861	49.103669
HF/TZVP	45.897014	45.813432	45.951305	45.881036	45.942284
HF/SVP	59.073237	59.013079	59.120616	59.042750	59.116501
MP2/SVP	86.781389	86.966208	86.599733	86.617879	86.941735

Monomer 15N NMR shielding constants of the nitrogen atoms

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(12,16)	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

Level	Average	H9	H11	H17	H20
B3LYP/TZVP	30.553719	30.253060	30.850568	30.895842	30.215404
BHLYP/TZVP	29.381975	28.993586	29.766352	29.805246	28.962466
CAM-B3LYP/TZVP	28.984064	28.624983	29.340204	29.374230	28.596552
wB97X-D/TZVP	28.665827	28.304313	29.024886	29.056704	28.277134
HF/TZVP	27.937050	27.375640	28.494279	28.522839	27.354902
HF/SVP	27.922430	27.448429	28.392464	28.416728	27.431463
MP2/SVP	30.180891	30.093267	30.268147	30.304807	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	H33
B3LYP/TZVP	30.850177	30.215437	30.900169	30.249095
BHLYP/TZVP	29.766070	28.961978	29.809293	28.990812
CAM-B3LYP/TZVP	29.340178	28.596066	29.377788	28.622511
wB97X-D/TZVP	29.024825	28.276702	29.060145	28.301908
HF/TZVP	28.494221	27.353003	28.526428	27.375090
HF/SVP	28.392238	27.430057	28.420366	27.447695
MP2/SVP	30.266422	30.059464	30.308990	30.088898
CASSCF/TZVP 14/14	27.5031	26.2656	27.5219	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

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

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

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

Monomer 15N NMR shielding constants of the nitrogen atoms

Level	Average(2,3)	N2	N3
B3LYP/TZVP	-15.568332	-15.557844	-15.578820
BHLYP/TZVP	2.910113	2.917094	2.903132
CAM-B3LYP/TZVP	-6.662562	-6.654002	-6.671122
wB97X-D/TZVP	-2.657330	-2.648540	-2.666120
HF/TZVP	31.956750	31.949431	31.964068
HF/SVP	56.356064	56.346214	56.365914
MP2/SVP	40.551510	40.587040	40.515979
CASSCF/TZVP 14/14	36.3585	36.4352	36.2818

Monomer 15N NMR shielding constants of the nitrogen atoms

Level	Average(5,6)	N5	N6	Average(2,3,5,6)
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	-4.882808	-5.765812
wB97X-D/TZVP	-0.924111	-0.911469	-0.936753	-1.790721
HF/TZVP	33.402190	33.418477	33.385902	32.679470
HF/SVP	57.704313	57.717212	57.691414	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

Level	Average	H6	H7	H25	H26
B3LYP/TZVP	28.978886	28.995852	28.246303	29.094575	28.995850
BHLYP/TZVP	28.981343	28.998500	28.250225	29.096133	28.998506
CAM-B3LYP/TZVP	27.654660	27.727797	26.914424	27.755056	27.727797
wB97X-D/TZVP	27.439136	27.529794	26.696939	27.529144	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

Monomer 1H NMR shielding constants in beta position

Level	H27	H28	H29	H30
B3LYP/TZVP	29.094574	29.578816	28.246303	29.578816
BHLYP/TZVP	29.096138	29.580504	28.250228	29.580510
CAM-B3LYP/TZVP	27.755056	28.221362	26.914424	28.221362
wB97X-D/TZVP	27.529144	28.000666	26.696939	28.000666
HF/TZVP	27.144952	27.597185	26.032549	27.597185
HF/SVP	27.146889	27.587522	26.134623	27.587522
MP2/SVP	28.478966	28.778383	27.861681	28.778383
CASSCF/TZVP 12/11	26.4060	26.5787	25.3265	26.5601
CASSCF/TZVP 12/12	26.9335	26.7626	26.1987	26.7626
CASSCF/TZVP 16/16	27.1992	27.1546	26.2282	27.1546

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

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

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	50.465969	44.593662	56.338269	56.338266	44.593677
BHLYP/TZVP	50.476513	44.600853	56.352165	56.352185	44.600848
CAM-B3LYP/TZVP	48.905438	40.981810	56.829064	56.829066	40.981810
wB97X-D/TZVP	51.727890	43.708200	59.747579	59.747581	43.708199
HF/TZVP	53.761489	41.520280	66.002698	66.002699	41.520280
HF/SVP	66.156681	55.294544	77.018817	77.018817	55.294544
MP2/SVP	86.863554	82.687380	91.039727	91.039727	82.687380
CASSCF/TZVP 12/11	59.4681	42.5946	79.7859	72.4654	43.0265
CASSCF/TZVP 12/12	69.6298	61.7331	77.5264	77.5264	61.7331
CASSCF/TZVP 16/16	73.6851	62.0098	85.3604	85.3604	62.0098

Monomer 15N NMR shielding constants of the nitrogen atoms with H

Level	Average	N8	N11
B3LYP/TZVP	17.504962	17.504975	17.504949
BHLYP/TZVP	7.4584270	17.458406	17.458448
CAM-B3LYP/TZVP	24.942908	24.942907	24.942908
wB97X-D/TZVP	28.769675	28.769675	28.769674
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 H

Level	Average	N1	N10
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

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

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

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

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

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

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

Level	Average	H9	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	24.243381	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	55.377785	56.822350	56.100068
BHLYP/TZVP	57.121683	59.028509	58.075096
CAM-B3LYP/TZVP	55.051095	56.826535	55.938815
wB97X-D/TZVP	57.518063	59.355701	58.436882
HF/TZVP	55.377785	56.822350	56.100068
HF/SVP	73.933327	76.260719	75.097023
MP2/SVP	88.142859	89.688051	88.915455
CASSCF/SVP 14/14	73.5690	75.2097	74.3894

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

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

Level	N2	N5	Average
B3LYP/TZVP	35.913449	32.715293	34.314371
BHLYP/TZVP	54.796619	50.127451	52.462035
CAM-B3LYP/TZVP	42.143007	38.329224	40.236116
wB97X-D/TZVP	44.548389	40.872840	42.710615
HF/TZVP	35.913449	32.715293	34.314371
HF/SVP	107.717453	102.266843	104.992148
MP2/SVP	80.423156	77.942535	79.182846
CASSCF/SVP 14/14	102.9626	97.4731	100.2179

S7 Cartesian coordinates of the molecular structures

Monomer or **1**

Ni	1.7345550	0.2053831	-0.1680936
F	6.4598840	-1.3871514	-2.2698142
F	6.3834863	-0.2270764	2.2826189
F	9.0036686	-0.7911953	2.4662908
F	10.3591021	-1.6568608	0.2893632
F	9.0796649	-1.9538618	-2.0777384
F	-2.1157530	1.8290029	3.0562672
F	-3.5156126	0.8275681	-1.3165970
N	3.2040829	1.2264695	-0.3333216
N	0.8532261	1.7699155	-0.1117331
C	4.8896229	-0.4786071	-0.1112682
N	0.2869345	-0.7955393	0.1968809
F	-6.0416672	1.4473436	-0.6454036
F	-6.6130195	2.2636504	1.8716691
C	8.3761126	-0.9331622	1.3090200
N	2.6406507	-1.3398888	-0.0234606
C	0.4944385	-2.0752463	0.4792742
C	-0.5539479	3.4483738	0.2870792
H	-1.4500526	4.0100334	0.5003924
C	2.8775927	-3.4558782	0.6094077
H	2.6467877	-4.4611957	0.9217248
C	1.5809029	2.8778987	-0.1525130
F	-4.6424081	2.4530193	3.7176639
C	3.9850898	-1.5566177	0.0286479
C	1.9499951	-2.4118356	0.3427457
C	-0.4517568	2.0252281	0.1874030
C	4.3260363	3.1414321	-0.2568455
H	4.5475365	4.1956411	-0.2251655
C	6.3441606	-0.7876213	-0.0003819
C	-3.0603724	1.7358119	2.1304968
C	-1.6520890	-1.5851855	0.9550288
H	-2.6822731	-1.6534382	1.2681981
C	-0.9849589	-0.4071337	0.4943322
C	-1.3390443	0.9619864	0.4719807
C	-3.7701720	1.2198317	-0.0760352
C	3.0368988	2.5414260	-0.2890742
C	-0.7317037	-2.6208181	0.9485017
H	-0.9105196	-3.6379471	1.2566474
C	4.5197498	0.8756549	-0.2786706
C	-4.3601207	2.0569066	2.4861187
C	-5.0764567	1.5388748	0.2561809
C	4.1421224	-2.9257182	0.4110948
H	5.0769812	-3.4487917	0.5392251
C	-2.7385193	1.3123493	0.8482739
C	8.4145141	-1.5307950	-1.0140256
C	0.7094240	3.9775342	0.0803939
H	0.9781997	5.0208496	0.1065811
C	7.0635932	-1.2369127	-1.0990488
C	5.2474052	2.1068365	-0.2545932
H	6.3206268	2.2128040	-0.2246618
C	9.0708167	-1.3779764	0.1961931
C	7.0260411	-0.6427571	1.1998076
C	-5.3700746	1.9582856	1.5432705

Dimer or $\mathbf{1}_2$

Ni	0.3671731	1.3275512	0.0000000
F	-1.1816182	0.9042232	5.3566523
F	2.4627793	3.6216580	4.0989818
F	2.7222191	4.4178782	6.6234801
F	1.0344388	3.4969754	8.5335554
F	-0.9235566	1.7421044	7.8657082
F	2.4627793	3.6216580	-4.0989818
F	-1.1816182	0.9042232	-5.3566523
N	1.6523192	1.0424741	1.2047193
N	1.6523192	1.0424741	-1.2047193
C	0.5184426	1.7588325	3.2053035

N	-0.8362037	1.8593789	-1.2122320
F	-0.9235566	1.7421044	-7.8657082
F	1.0344388	3.4969754	-8.5335554
C	1.7767657	3.5449386	6.3076398
N	-0.8362037	1.8593789	1.2122320
C	-1.9812439	2.3841373	-0.7163083
C	2.9987338	0.8632031	-2.9674699
H	3.3555228	0.8662682	-3.9849843
C	-2.6944378	2.9406427	1.8395433
H	-3.6547983	3.4297084	1.8089378
C	2.8595623	0.6690112	-0.7168114
F	2.7222191	4.4178782	-6.6234801
C	-0.6976105	2.0662059	2.5306242
C	-1.9812439	2.3841373	0.7163083
C	1.6551134	1.2211477	-2.5347617
C	3.7284738	0.5324131	1.8587791
H	4.7647464	0.2355982	1.8419980
C	0.6547029	2.1926036	4.6196443
C	1.6373533	3.1057339	-5.0013491
C	-1.9151763	2.7522002	-2.9457138
H	-2.1566814	3.0617027	-3.9498767
C	-0.6976105	2.0662059	-2.5306242
C	0.5184426	1.7588325	-3.2053035
C	-0.2064107	1.7681669	-5.6270918
C	2.8595623	0.6690112	0.7168114
C	-2.6944378	2.9406427	-1.8395433
H	-3.6547983	3.4297084	-1.8089378
C	1.6551134	1.2211477	2.5347617
C	1.7767657	3.5449386	-6.3076398
C	-0.0892127	2.1927388	-6.9388689
C	-1.9151763	2.7522002	2.9457138
H	-2.1566814	3.0617027	3.9498767
C	0.6547029	2.1926036	-4.6196443
C	-0.0892127	2.1927388	6.9388689
C	3.7284738	0.5324131	-1.8587791
H	4.7647464	0.2355982	-1.8419980
C	-0.2064107	1.7681669	5.6270918
C	2.9987338	0.8632031	2.9674699
H	3.3555228	0.8662682	3.9849843
C	0.9114634	3.0840072	7.2840258
C	1.6373533	3.1057339	5.0013491
C	0.9114634	3.0840072	-7.2840258
Ni	-0.3671731	-1.3275512	0.0000000
F	1.1816182	-0.9042232	-5.3566523
F	-2.4627793	-3.6216580	-4.0989818
F	-2.7222191	-4.4178782	-6.6234801
F	-1.0344388	-3.4969754	-8.5335554
F	0.9235566	-1.7421044	-7.8657082
F	-2.4627793	-3.6216580	4.0989818
F	1.1816182	-0.9042232	5.3566523
N	-1.6523192	-1.0424741	-1.2047193
N	-1.6523192	-1.0424741	1.2047193
C	-0.5184426	-1.7588325	-3.2053035
N	0.8362037	-1.8593789	1.2122320
F	0.9235566	-1.7421044	7.8657082
F	-1.0344388	-3.4969754	8.5335554
C	-1.7767657	-3.5449386	-6.3076398
N	0.8362037	-1.8593789	-1.2122320
C	1.9812439	-2.3841373	0.7163083
C	-2.9987338	-0.8632031	2.9674699
H	-3.3555228	-0.8662682	3.9849843
C	2.6944378	-2.9406427	-1.8395433
H	3.6547983	-3.4297084	-1.8089378
C	-2.8595623	-0.6690112	0.7168114
F	-2.7222191	-4.4178782	6.6234801
C	0.6976105	-2.0662059	-2.5306242
C	1.9812439	-2.3841373	-0.7163083
C	-1.6551134	-1.2211477	2.5347617
C	-3.7284738	-0.5324131	-1.8587791

H	-4.7647464	-0.2355982	-1.8419980
C	-0.6547029	-2.1926036	-4.6196443
C	-1.6373533	-3.1057339	5.0013491
C	1.9151763	-2.7522002	2.9457138
H	2.1566814	-3.0617027	3.9498767
C	0.6976105	-2.0662059	2.5306242
C	-0.5184426	-1.7588325	3.2053035
C	0.2064107	-1.7681669	5.6270918
C	-2.8595623	-0.6690112	-0.7168114
C	2.6944378	-2.9406427	1.8395433
H	3.6547983	-3.4297084	1.8089378
C	-1.6551134	-1.2211477	-2.5347617
C	-1.7767657	-3.5449386	6.3076398
C	0.0892127	-2.1927388	6.9388689
C	1.9151763	-2.7522002	-2.9457138
H	2.1566814	-3.0617027	-3.9498767
C	-0.6547029	-2.1926036	4.6196443
C	0.0892127	-2.1927388	-6.9388689
C	-3.7284738	-0.5324131	1.8587791
H	-4.7647464	-0.2355982	1.8419980
C	0.2064107	-1.7681669	-5.6270918
C	-2.9987338	-0.8632031	-2.9674699
H	-3.3555228	-0.8662682	-3.9849843
C	-0.9114634	-3.0840072	-7.2840258
C	-1.6373533	-3.1057339	-5.0013491
C	-0.9114634	-3.0840072	7.2840258

Phenyl-substituted dimer with C_2 symmetry or $\mathbf{2}_2$

Ni	-1.1544643	-0.8711229	0.0120983
H	0.1457191	-1.5440709	5.2249419
H	-3.8620005	-0.2115500	4.5410863
H	-4.3105787	-0.3202600	6.9573109
H	-2.5447573	-1.0904190	8.5177239
H	-0.3118299	-1.7066288	7.6293046
H	-3.3889821	-0.9523312	-4.8456332
H	0.7854324	-1.8588925	-4.9011152
N	-2.0580748	0.2226513	1.1160989
N	-1.9249232	0.0749982	-1.3005578
C	-1.5613038	-0.8331546	3.2510013
N	-0.4318307	-2.0852857	-1.1056461
H	0.7221470	-2.0356188	-7.3540894
H	-1.4020704	-1.6529137	-8.5728492
C	-3.3333048	-0.5934915	6.5797017
N	-0.5569384	-1.9332892	1.3345267
C	0.0637760	-3.2027685	-0.5142559
C	-2.5847683	1.0651820	-3.1882718
H	-2.7452805	1.2810848	-4.2299319
C	0.0740989	-3.9303854	2.1193217
H	0.4637254	-4.9342845	2.1604436
C	-2.5958965	1.1737241	-0.9241443
H	-3.4616669	-1.1174139	-7.3014472
C	-0.8513993	-1.9028558	2.6703125
C	-0.0394944	-3.1063443	0.9413256
C	-1.8715468	-0.0867040	-2.6547428
C	-3.1278074	2.1156717	1.5869277
H	-3.6452992	3.0559348	1.4889699
C	-1.8262151	-0.8793209	4.6994009
C	-2.4844735	-1.1656091	-5.3977937
C	-0.0670552	-3.5320281	-2.7530340
H	-0.0174576	-3.9787572	-3.7318476
C	-0.5628137	-2.2205079	-2.4426864
C	-1.2315139	-1.1994056	-3.2335260
C	-0.1439994	-1.7090055	-5.4265225
C	-2.6623870	1.2878929	0.5330763
C	0.3210378	-4.1356520	-1.5565512
H	0.7188670	-5.1312710	-1.4447263
C	-2.1067259	0.2651424	2.4654540
C	-2.5247596	-1.2704807	-6.7808812
C	-0.1832012	-1.8047825	-6.8082639

C	-0.4267636	-3.2034166	3.1728869
H	-0.5150450	-3.5475969	4.1890401
C	-1.2886768	-1.3673247	-4.6967893
C	-1.0976997	-1.3883954	6.9570048
C	-3.0284716	1.8277124	-2.1302144
H	-3.5789975	2.7510599	-2.1943955
C	-0.8403395	-1.3104985	5.5972242
C	-2.7842981	1.4856163	2.7879027
H	-2.9808305	1.8653743	3.7757094
C	-2.3441086	-1.0299168	7.4558787
C	-3.0787698	-0.5194505	5.2184266
C	-1.3722535	-1.5811183	-7.4931830
Ni	1.1544643	0.8711229	0.0120983
H	-0.7854324	1.8588925	-4.9011152
H	3.3889821	0.9523312	-4.8456332
H	3.4616669	1.1174139	-7.3014472
H	1.4020704	1.6529137	-8.5728492
H	-0.7221470	2.0356188	-7.3540894
H	3.8620005	0.2115500	4.5410863
H	-0.1457191	1.5440709	5.2249419
N	1.9249232	-0.0749982	-1.3005578
N	2.0580748	-0.2226513	1.1160989
C	1.2315139	1.1994056	-3.2335260
N	0.5569384	1.9332892	1.3345267
H	0.3118299	1.7066288	7.6293046
H	2.5447573	1.0904190	8.5177239
C	2.5247596	1.2704807	-6.7808812
N	0.4318307	2.0852857	-1.1056461
C	0.0394944	3.1063443	0.9413256
C	2.7842981	-1.4856163	2.7879027
H	2.9808305	-1.8653743	3.7757094
C	-0.3210378	4.1356520	-1.5565512
H	-0.7188670	5.1312710	-1.4447263
C	2.6623870	-1.2878929	0.5330763
H	4.3105787	0.3202600	6.9573109
C	0.5628137	2.2205079	-2.4426864
C	-0.0637760	3.2027685	-0.5142559
C	2.1067259	-0.2651424	2.4654540
C	3.0284716	-1.8277124	-2.1302144
H	3.5789975	-2.7510599	-2.1943955
C	1.2886768	1.3673247	-4.6967893
C	3.0787698	0.5194505	5.2184266
C	0.4267636	3.2034166	3.1728869
H	0.5150450	3.5475969	4.1890401
C	0.8513993	1.9028558	2.6703125
C	1.5613038	0.8331546	3.2510013
C	0.8403395	1.3104985	5.5972242
C	2.5958965	-1.1737241	-0.9241443
C	-0.0740989	3.9303854	2.1193217
H	-0.4637254	4.9342845	2.1604436
C	1.8715468	0.0867040	-2.6547428
C	3.3333048	0.5934915	6.5797017
C	1.0976997	1.3883954	6.9570048
C	0.0670552	3.5320281	-2.7530340
H	0.0174576	3.9787572	-3.7318476
C	1.8262151	0.8793209	4.6994009
C	0.1832012	1.8047825	-6.8082639
C	3.1278074	-2.1156717	1.5869277
H	3.6452992	-3.0559348	1.4889699
C	0.1439994	1.7090055	-5.4265225
C	2.5847683	-1.0651820	-3.1882718
H	2.7452805	-1.2810848	-4.2299319
C	1.3722535	1.5811183	-7.4931830
C	2.4844735	1.1656091	-5.3977937
C	2.3441086	1.0299168	7.4558787

Monomer without pentafluorophenyl groups or **1′**

Ni	-0.0000123	0.1036975	0.4184611
N	1.2122121	-1.2067988	0.6247207

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

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

Ni	-1.3631938	-0.1972603	0.0000000
N	-1.6185891	1.0941124	1.2047196
N	-1.6185891	1.0941124	-1.2047196
C	-1.8189081	-0.2320544	3.2053042
N	-1.3666084	-1.5129143	-1.2122323
N	-1.3666084	-1.5129143	1.2122323
C	-1.3869924	-2.7723084	-0.7163085
C	-1.9954924	2.3990703	-2.9674705
H	-2.1416763	2.7245516	-3.9849851
C	-1.6099866	-3.6490169	1.8395437
H	-1.6719010	-4.7249559	1.8089382
C	-1.7617434	2.3496673	-0.7168116
C	-1.6116950	-1.4691183	2.5306247
C	-1.3869924	-2.7723084	0.7163085
C	-1.7833240	1.0248703	-2.5347622
C	-1.9858358	3.2002254	1.8587795
H	-2.1304718	4.2684206	1.8419984
H	-2.0207841	-0.2483307	4.2667731
C	-1.7505786	-2.8597177	-2.9457144
H	-1.9369414	-3.2052398	-3.9498775
C	-1.6116950	-1.4691183	-2.5306247
C	-1.8189081	-0.2320544	-3.2053042
C	-1.7617434	2.3496673	0.7168116
C	-1.6099866	-3.6490169	-1.8395437
H	-1.6719010	-4.7249559	-1.8089382
C	-1.7833240	1.0248703	2.5347622
C	-1.7505786	-2.8597177	2.9457144
H	-1.9369414	-3.2052398	3.9498775
H	-2.0207841	-0.2483307	-4.2667731
C	-1.9858358	3.2002254	-1.8587795
H	-2.1304718	4.2684206	-1.8419984
C	-1.9954924	2.3990703	2.9674705
H	-2.1416763	2.7245516	3.9849851
Ni	1.3631938	0.1972603	0.0000000
N	1.6185891	-1.0941124	-1.2047196
N	1.6185891	-1.0941124	1.2047196

C	1.8189081	0.2320544	-3.2053042
N	1.3666084	1.5129143	1.2122323
N	1.3666084	1.5129143	-1.2122323
C	1.3869924	2.7723084	0.7163085
C	1.9954924	-2.3990703	2.9674705
H	2.1416763	-2.7245516	3.9849851
C	1.6099866	3.6490169	-1.8395437
H	1.6719010	4.7249559	-1.8089382
C	1.7617434	-2.3496673	0.7168116
C	1.6116950	1.4691183	-2.5306247
C	1.3869924	2.7723084	-0.7163085
C	1.7833240	-1.0248703	2.5347622
C	1.9858358	-3.2002254	-1.8587795
H	2.1304718	-4.2684206	-1.8419984
H	2.0207841	0.2483307	-4.2667731
C	1.7505786	2.8597177	2.9457144
H	1.9369414	3.2052398	3.9498775
C	1.6116950	1.4691183	2.5306247
C	1.8189081	0.2320544	3.2053042
C	1.7617434	-2.3496673	-0.7168116
C	1.6099866	3.6490169	1.8395437
H	1.6719010	4.7249559	1.8089382
C	1.7833240	-1.0248703	-2.5347622
C	1.7505786	2.8597177	-2.9457144
H	1.9369414	3.2052398	-3.9498775
H	2.0207841	0.2483307	4.2667731
C	1.9858358	-3.2002254	1.8587795
H	2.1304718	-4.2684206	1.8419984
C	1.9954924	-2.3990703	-2.9674705
H	2.1416763	-2.7245516	-3.9849851

Free-base norcorrole

N	1.7144615	-0.0132479	-0.0000178
C	2.2597758	-1.2077326	-0.0000305
C	2.6914494	0.9646455	-0.0000198
C	3.7052271	-1.0725094	-0.0000410
C	3.9701805	0.2766725	-0.0000237
H	4.4271082	-1.8737306	-0.0000680
H	4.9447287	0.7404625	-0.0000098
N	0.0038355	-1.8187918	0.0000054
H	-0.2829471	-0.8389987	0.0000197
N	-1.7144615	0.0132479	0.0000119
N	-0.0038355	1.8187918	-0.0000001
H	0.2829470	0.8389987	-0.0000202
C	-0.9650363	-2.7659511	0.0000195
C	-2.2597758	1.2077326	-0.0000009
C	0.9650363	2.7659511	0.0000110
C	1.2532163	-2.2997280	-0.0000180
C	-2.6914494	-0.9646455	0.0000043
C	-1.2532163	2.2997280	0.0000178
C	-0.2650645	-3.9976949	0.0000026
C	-3.7052271	1.0725094	-0.0000166
C	0.2650645	3.9976949	0.0000357
C	1.1165422	-3.7048195	0.0000501
C	-3.9701805	-0.2766725	-0.0000314
C	-1.1165422	3.7048195	0.0000181
H	-0.7033329	-4.9826235	-0.0000619
H	-4.4271082	1.8737306	-0.0000099
H	0.7033329	4.9826235	0.0000692
H	1.9166348	-4.4262251	0.0001568
H	-4.9447287	-0.7404625	-0.0000726
H	-1.9166348	4.4262251	-0.0000006
C	-2.3278689	-2.3078129	0.0000164
C	2.3278689	2.3078129	-0.0000064
H	-3.1120492	-3.0549562	0.0000264
H	3.1120492	3.0549562	-0.0000157