Electronic Supplementary Material (ESI) for RSC Advances.

Metamagentism and canted antiferromagnetic ordering in two monomeric Co^{II} complexes with 1-(2pyrimidyl)piperazine. Hirshfeld surface analysis and theoretical studies

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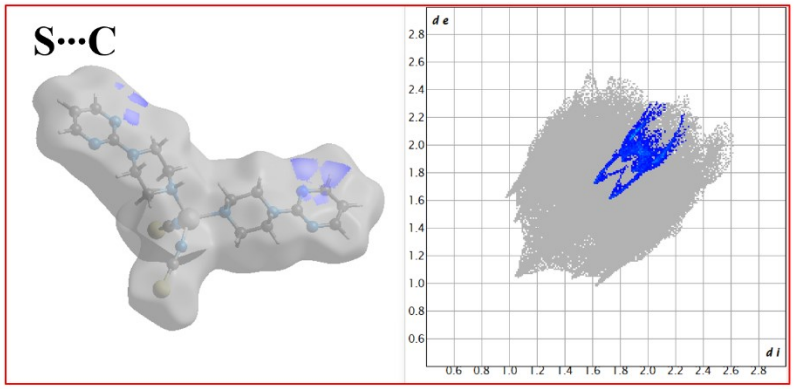
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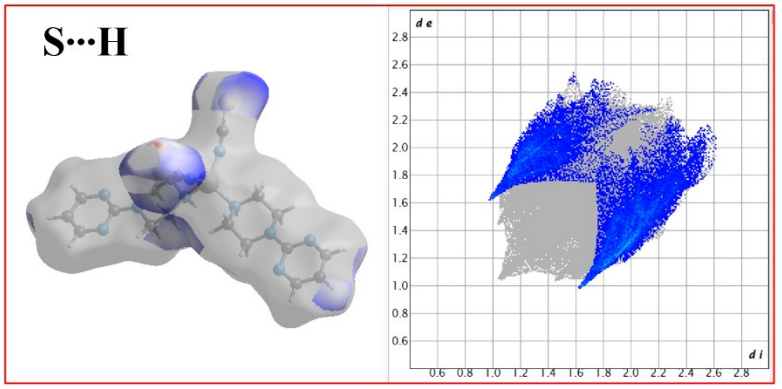
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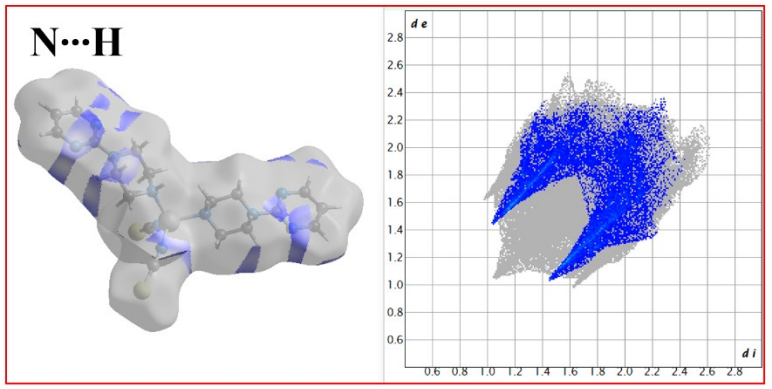
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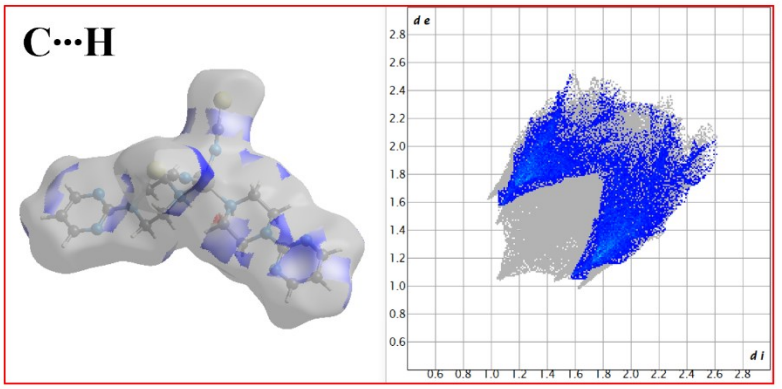
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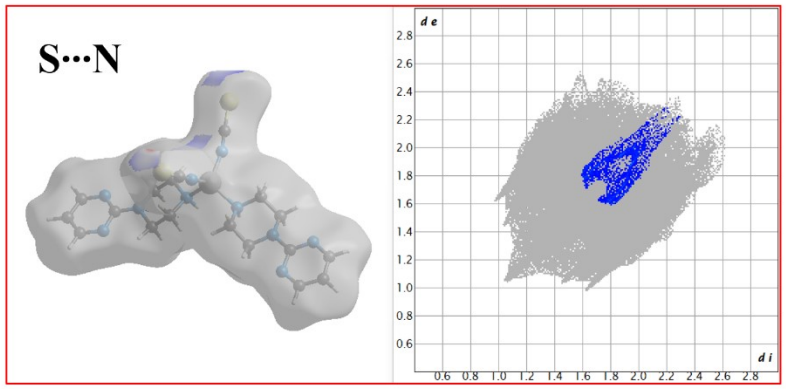
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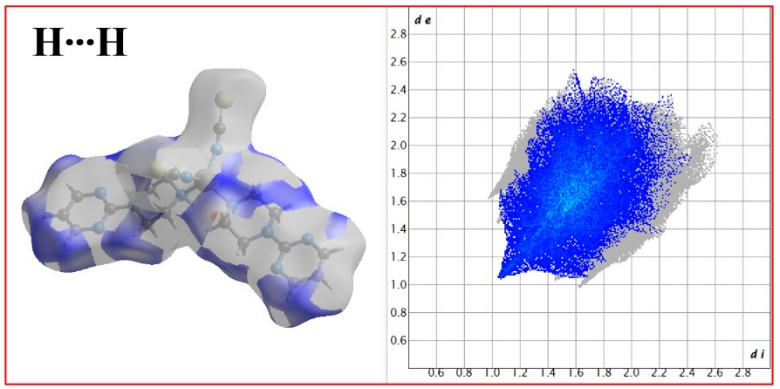
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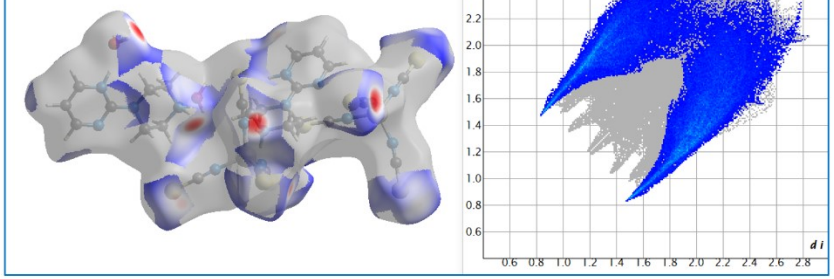

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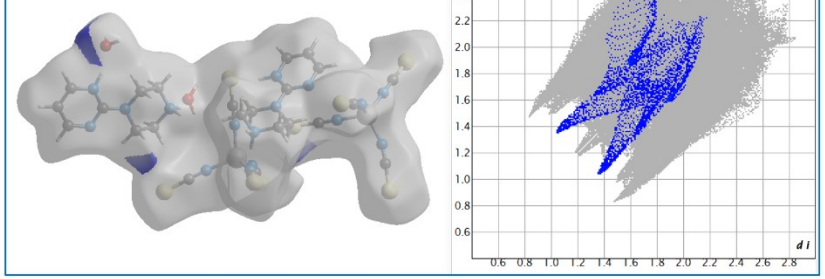

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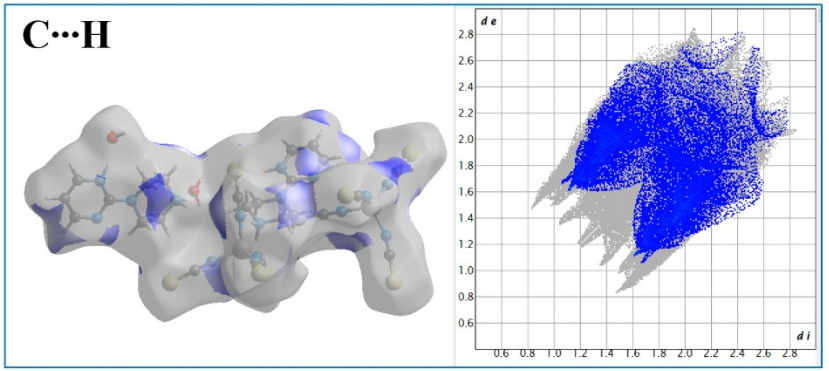

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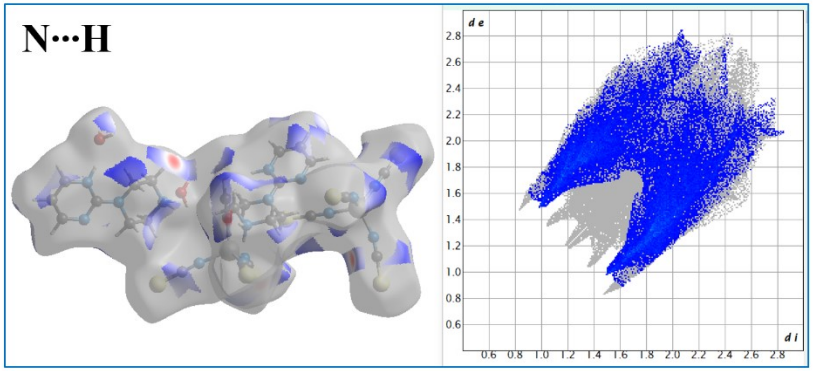

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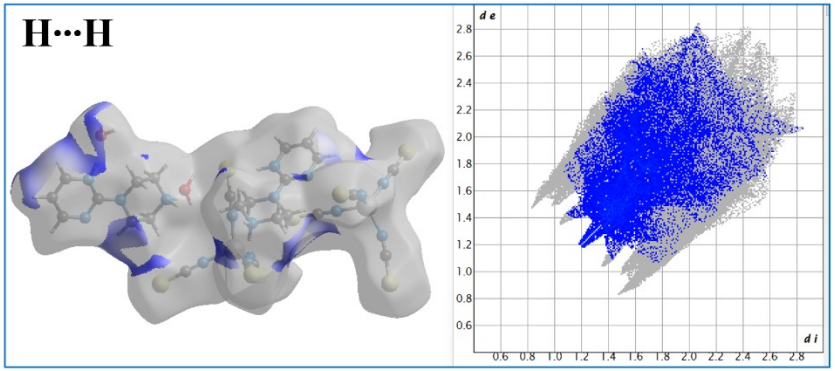
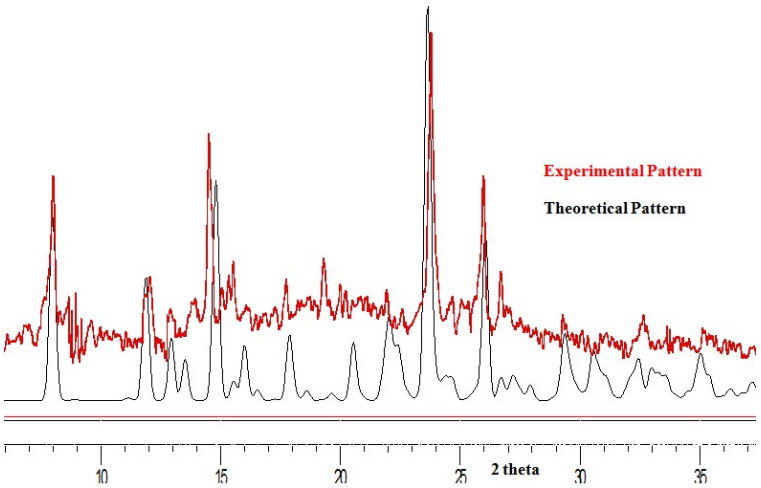


Figure S1: The decomposed d_{norm} maps and their fingerprint plots of both complexes.

Compound 1:



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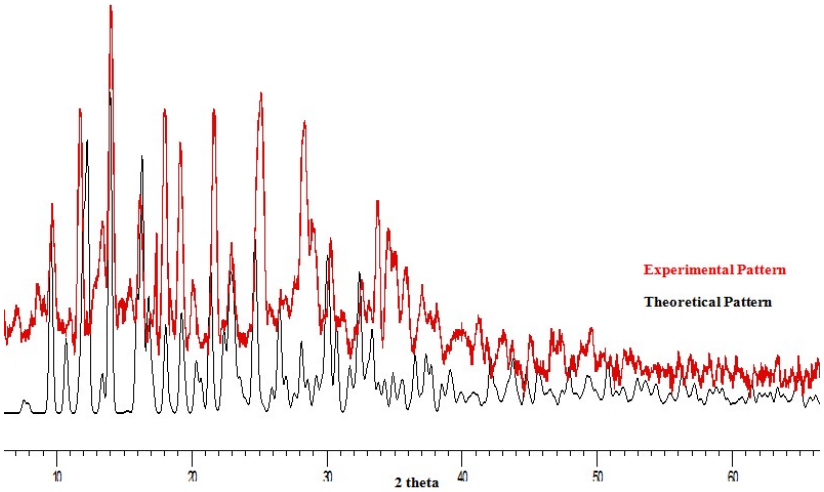

Fig S2. The XRPD of the two compounds

Table S1: The enrichment contacts ratio of both complexes

Complex-I							
E	H	C	N	S	Co	HC	
H	0						
C	0.02	0.78					
N	0	**1.52**	0.37				
S	**5.74**	0.67	0.39	0.31			
Co	0	0.35	0	**3.58**	0		
HC	0.18	**1.21**	**1.2**	**1.04**	0.74	0.93	
Complex-II							
E	H	C	N	O	S	Co	HC
H	0						
C	0.61	**1.23**					
N	0.29	0.87	0.66				
O	0	0.52	0.04	0			
S	**2.22**	0.89	**1.34**	0.06	0.39		
Co	0.3	0.98	0.14	0	**1.48**		0
HC	0.39	**1.16**	**1.24**	**3.56**	**1.33**	**1.12**	0.42

Table S2: Topological properties of metal complex 1

Atom1	Atom2	Gcp kJ/mol/Bohr^3	Vcp kJ/mol/Bohr^3	DIST12	$\rho_{(r)}$	$\nabla^2\rho_{(r)}$	λ1	λ2	λ3	ε
Co1	N1	233.89	-260.11	2.0374	0.49053	7.625	-2.072	-2.06	11.757	0.0057
Co1	N13	295.53	-335.14	1.9546	0.5765	9.396	-2.71	-2.71	14.816	0
Co1	N15	308.05	-350.76	1.9419	0.59362	9.742	-2.826	-2.826	15.393	0.0001
Co1	N1A	230.39	-255.86	2.0417	0.48537	7.524	-2.037	-2.035	11.596	0.0012
S1	C14	449.15	-941.99	1.6247	1.29014	-1.604	-4.979	-4.979	8.354	0
S2	C16	447.19	-935.96	1.6275	1.28468	-1.526	-4.959	-4.959	8.391	0
N1	H1	562.04	-1780.76	0.8893	2.00809	-24.11	-27.781	-27.736	31.406	0.0016
N1	C2	620.01	-1159.78	1.4777	1.42809	2.947	-7.01	-6.976	16.932	0.0048
N1	C6	611.76	-1138.65	1.484	1.41088	3.116	-6.931	-6.874	16.921	0.0084
N4	C3	635.25	-1204.28	1.4598	1.46496	2.432	-7.274	-7.27	16.975	0.0006
N4	C5	636.85	-1208.37	1.4588	1.46822	2.399	-7.334	-7.235	16.967	0.0137
N4	C7	712.6	-1455.77	1.3812	1.6668	-1.122	-8.553	-8.352	15.783	0.024
N8	C7	755.05	-1605.86	1.3413	1.78141	-3.515	-9.16	-8.865	14.51	0.0333
N8	C9	773.51	-1651.67	1.3339	1.81305	-3.842	-9.246	-9.053	14.457	0.0213
N12	C7	745.69	-1572.3	1.3499	1.75616	-2.971	-9.008	-8.784	14.822	0.0255
N12	C11	764.88	-1623.18	1.3406	1.79219	-3.43	-9.156	-8.97	14.695	0.0207
N13	C14	1419.45	-2601.33	1.1642	2.30819	8.723	-12.764	-12.763	34.25	0
N15	C16	1466.06	-2654.35	1.158	2.32988	10.199	-13.033	-13.033	36.265	0.0001
N1A	H1A	560.96	-1698.63	0.9058	1.94181	-21.174	-25.899	-25.849	30.575	0.0019
N1A	C2A	605.7	-1122.57	1.4893	1.39757	3.261	-6.85	-6.794	16.906	0.0082
N1A	C6A	626.5	-1177.69	1.4715	1.44283	2.765	-7.113	-7.066	16.943	0.0066
N4A	C3A	647.68	-1237.45	1.4504	1.49152	2.126	-7.411	-7.411	16.948	0
N4A	C5A	632.76	-1197	1.4623	1.45898	2.515	-7.252	-7.213	16.98	0.0054
N4A	C7A	727.57	-1506.14	1.3677	1.70551	-1.872	-8.798	-8.508	15.434	0.034
N8A	C7A	744.86	-1568.11	1.3513	1.75284	-2.878	-8.986	-8.769	14.876	0.0248

N8A	C9A	784.39	-1688.56	1.3249	1.83997	-4.398	-9.408	-9.114	14.124	0.0323
N12A	C7A	754.03	-1600.93	1.3427	1.77756	-3.41	-9.074	-8.913	14.577	0.0181
N12A	C11A	776.22	-1661.31	1.3314	1.82017	-3.997	-9.327	-9.033	14.363	0.0326
C2	H2A	435.25	-1107.71	0.9895	1.46836	-8.709	-12.027	-12.018	15.336	0.0007
C2	H2B	435.13	-1107.37	0.9896	1.46809	-8.705	-12.027	-12.015	15.336	0.001
C2	C3	470.5	-913.05	1.5091	1.24691	1.026	-5.494	-5.491	12.011	0.0005
C3	H3A	433.69	-1103.2	0.9905	1.46467	-8.658	-11.998	-11.995	15.335	0.0003
C3	H3B	434.06	-1104.14	0.9902	1.46542	-8.666	-12.003	-11.996	15.334	0.0006
C5	H5A	433.72	-1102.69	0.9907	1.46414	-8.637	-11.99	-11.976	15.329	0.0012
C5	H5B	433.97	-1104.87	0.9898	1.46618	-8.699	-12.022	-12.012	15.336	0.0009
C5	C6	464.63	-897.94	1.5153	1.23342	1.15	-5.427	-5.42	11.996	0.0013
C6	H6A	435	-1106.41	0.99	1.4672	-8.68	-12.005	-12.003	15.328	0.0001
C6	H6B	435.3	-1107.84	0.9894	1.46846	-8.71	-12.02	-12.02	15.33	0
C9	H9	455.46	-1213.99	0.9497	1.56159	-11.127	-13.317	-13.141	15.331	0.0133
C9	C10	591.95	-1271.1	1.3721	1.551	-3.202	-7.337	-7.114	11.249	0.0312
C10	H10	455.78	-1214.55	0.9501	1.56197	-11.124	-13.236	-13.229	15.341	0.0006
C10	C11	588.34	-1260.32	1.3754	1.54241	-3.07	-7.318	-7.044	11.292	0.0389
C11	H11	454.77	-1211.81	0.9501	1.55985	-11.097	-13.23	-13.19	15.323	0.0031
C2A	H2A1	435.07	-1106.39	0.9901	1.46714	-8.674	-12.006	-11.997	15.329	0.0008
C2A	H2A2	435.11	-1106.54	0.9901	1.46727	-8.676	-12.01	-11.997	15.33	0.0011
C2A	C3A	473.52	-920.89	1.5059	1.25388	0.96	-5.533	-5.524	12.016	0.0015
C3A	H3A1	433.81	-1103.24	0.9906	1.46464	-8.651	-11.998	-11.993	15.341	0.0004
C3A	H3A2	435.12	-1107.58	0.9893	1.46829	-8.714	-12.033	-12.023	15.342	0.0008
C5A	H5A1	434.06	-1104.55	0.99	1.46582	-8.681	-12.011	-12.003	15.333	0.0006
C5A	H5A2	433.87	-1104.55	0.9898	1.46592	-8.695	-12.019	-12.011	15.336	0.0007
C5A	C6A	471.84	-916.47	1.5078	1.24994	0.999	-5.51	-5.504	12.013	0.001
C6A	H6A1	434.64	-1104.78	0.9906	1.46576	-8.646	-11.998	-11.984	15.335	0.0012
C6A	H6A2	435.24	-1106.97	0.9899	1.46763	-8.683	-12.014	-12.005	15.336	0.0007
C9A	H9A	455.3	-1212.56	0.9503	1.56031	-11.086	-13.244	-13.18	15.338	0.0049
C9A	C10A	588.38	-1259.93	1.3757	1.54202	-3.054	-7.281	-7.072	11.3	0.0295
C10A	H10A	456.2	-1217.11	0.9491	1.56421	-11.188	-13.33	-13.192	15.334	0.0105
C10A	C11A	587.44	-1257.24	1.3765	1.53989	-3.024	-7.284	-7.048	11.308	0.0336

C11A	H11A	455	-1212.23	0.9501	1.56014	-11.096	-13.214	-13.212	15.33	0.0002
H6A	H2A2	12.08	-10.43	2.3798	0.06066	0.504	-0.164	-0.115	0.783	0.4205

Table S3: Topological properties of metal complex 2

Atom1	Atom2	Gcp kJ/mol/Bohr^3	Vcp kJ/mol/Bohr^3	DIST12	$\rho_{(r)}$	$\nabla^2\rho_{(r)}$	λ1	λ2	λ3	ε
Co1	N13	294.86	-334.23	1.955	0.57544	9.38	-2.711	-2.71	14.801	0.0002
Co1	N15	291.35	-329.88	1.9589	0.57064	9.282	-2.675	-2.675	14.633	0.0001
Co1	N17	293.22	-332.21	1.9571	0.57322	9.334	-2.691	-2.69	14.715	0.0003
Co1	N19	288.76	-326.68	1.9615	0.56708	9.21	-2.652	-2.652	14.513	0.0001
S1	C14	446.76	-934.66	1.6281	1.28351	-1.51	-4.955	-4.955	8.399	0
S2	C16	439.58	-913.18	1.6377	1.26404	-1.249	-4.884	-4.884	8.518	0
S3	C18	439.27	-912.19	1.6382	1.26312	-1.235	-4.88	-4.88	8.524	0
S4	C20	446.06	-932.63	1.6289	1.28169	-1.487	-4.948	-4.948	8.409	0
N13	C14	1475.16	-2664.55	1.1567	2.33399	10.492	-13.089	-13.089	36.67	0
N15	C16	1420.03	-2601.39	1.1641	2.30803	8.762	-12.768	-12.767	34.297	0.0001
N17	C18	1427.81	-2610.33	1.1631	2.31172	9.006	-12.811	-12.81	34.626	0.0001
N19	C20	1391.08	-2568.82	1.168	2.29475	7.833	-12.602	-12.602	33.037	0
Co1A	N13A	299.34	-339.84	1.9507	0.58166	9.503	-2.748	-2.746	14.997	0.001
Co1A	N15A	289.42	-327.48	1.9611	0.56796	9.229	-2.657	-2.656	14.541	0.0003
Co1A	N17A	305.03	-346.97	1.9449	0.58947	9.659	-2.8	-2.799	15.258	0.0002
Co1A	N19A	295.83	-335.48	1.9543	0.57686	9.406	-2.715	-2.714	14.835	0.0001
S1A	C14A	442.73	-922.51	1.6335	1.2725	-1.36	-4.914	-4.914	8.469	0
S2A	C16A	439.53	-912.79	1.638	1.26364	-1.239	-4.881	-4.88	8.523	0.0002
S3A	C18A	440.81	-916.19	1.6367	1.26666	-1.269	-4.891	-4.888	8.509	0.0007
S4A	C20A	438.99	-911	1.639	1.26197	-1.212	-4.874	-4.874	8.536	0.0002
N13A	C14A	1477.71	-2667.29	1.1564	2.33505	10.579	-13.102	-13.102	36.784	0
N15A	C16A	1477.94	-2667.38	1.1564	2.33504	10.592	-13.104	-13.103	36.798	0.0001
N17A	C18A	1587.21	-2792.11	1.1423	2.38559	14.037	-13.759	-13.758	41.553	0.0001

N19A	C20A	1620.69	-2830.24	1.1381	2.40088	15.096	-13.966	-13.965	43.026	0
N4	C3	633.65	-1199.84	1.4613	1.46135	2.477	-7.29	-7.211	16.978	0.0109
N4	C5	638.3	-1211.7	1.4582	1.4708	2.383	-7.332	-7.253	16.968	0.0108
N4	C7	758.84	-1613.54	1.3402	1.78643	-3.519	-9.178	-8.886	14.545	0.0329
N1	H1A	563.88	-1752.26	0.8965	1.98436	-22.929	-27.047	-27.042	31.16	0.0002
N1	H1B	562.26	-1689.7	0.9096	1.93393	-20.751	-25.635	-25.606	30.49	0.0011
N1	C2	612.83	-1138.84	1.4865	1.41053	3.187	-6.861	-6.853	16.901	0.0012
N1	C6	613.42	-1141	1.485	1.41242	3.152	-6.884	-6.881	16.918	0.0004
N8	C7	760.13	-1616.22	1.3399	1.7882	-3.523	-9.185	-8.868	14.53	0.0358
N8	C9	792.26	-1716.18	1.318	1.86007	-4.834	-9.491	-9.196	13.853	0.032
N12	H12	559.75	-1782.72	0.8877	2.01058	-24.35	-28.028	-27.893	31.571	0.0048
N12	C7	750.47	-1580.69	1.3507	1.76143	-2.928	-9.035	-8.738	14.845	0.0339
N12	C11	756.74	-1584.92	1.3542	1.76238	-2.623	-9.04	-8.696	15.113	0.0395
C2	H2A	434.2	-1105.92	0.9894	1.46711	-8.721	-12.029	-12.022	15.331	0.0006
C2	H2B	433.81	-1104.37	0.9899	1.46577	-8.693	-12.014	-12.008	15.33	0.0005
C2	C3	465	-898.85	1.5149	1.23423	1.144	-5.427	-5.426	11.997	0.0001
C3	H3A	434.26	-1105.82	0.9895	1.46698	-8.712	-12.03	-12.016	15.334	0.0012
C3	H3B	434.33	-1104.24	0.9904	1.46538	-8.649	-11.99	-11.986	15.327	0.0003
C5	H5A	435.15	-1107.45	0.9893	1.46815	-8.707	-12.024	-12.019	15.336	0.0005
C5	H5B	433.49	-1102.12	0.9909	1.46369	-8.633	-11.99	-11.977	15.334	0.0011
C5	C6	470.22	-912.31	1.5093	1.24625	1.033	-5.488	-5.488	12.009	0
C6	H6A	433.89	-1105.12	0.9896	1.46647	-8.714	-12.025	-12.021	15.332	0.0003
C6	H6B	433.57	-1103.33	0.9903	1.46485	-8.672	-12.003	-11.997	15.328	0.0005
C9	H9	455.18	-1211.74	0.9505	1.55959	-11.065	-13.276	-13.121	15.331	0.0118
C9	C10	572.62	-1211.44	1.3918	1.50278	-2.431	-7.096	-6.836	11.502	0.038
C10	H10	456.17	-1215.19	0.9501	1.5624	-11.119	-13.314	-13.158	15.354	0.0119
C10	C11	621.18	-1362.11	1.3439	1.6228	-4.396	-7.739	-7.461	10.804	0.0373
C11	H11	455.25	-1212.76	0.9502	1.56052	-	-13.272	-13.16	15.335	0.0085

						11.097				
N4A	C3A	635.65	-1204.91	1.4599	1.46539	2.437	-7.312	-7.224	16.973	0.0123
N4A	C5A	638.46	-1211.82	1.4583	1.47084	2.39	-7.32	-7.263	16.973	0.0077
N4A	C7A	757.06	-1608.02	1.3415	1.78241	-3.447	-9.087	-8.94	14.58	0.0164
N1A	H1C	562.11	-1714.67	0.9041	1.95449	-21.678	-26.234	-26.213	30.769	0.0008
N1A	H1D	566.78	-1731.78	0.9019	1.96655	-21.963	-26.437	-26.434	30.908	0.0001
N1A	C2A	624.15	-1169.97	1.4753	1.43626	2.876	-7.033	-7.032	16.94	0.0001
N1A	C6A	596.58	-1096.52	1.5002	1.37547	3.548	-6.659	-6.648	16.855	0.0016
N8A	C7A	755.68	-1602.44	1.343	1.77816	-3.344	-9.057	-8.92	14.633	0.0153
N8A	C9A	785.61	-1694.19	1.3232	1.84424	-4.515	-9.367	-9.2	14.053	0.0182
N12A	H12A	557.28	-1874.04	0.8701	2.08399	-27.884	-30.204	-30.156	32.476	0.0016
N12A	C7A	744.96	-1562.48	1.3552	1.74784	-2.664	-8.832	-8.819	14.987	0.0016
N12A	C11A	765.2	-1613.66	1.3473	1.78378	-3.057	-8.98	-8.934	14.857	0.0051
C2A	H2C	433.72	-1103.79	0.9901	1.46524	-8.678	-12.005	-12.004	15.331	0.0001
C2A	H2D	433.42	-1103	0.9903	1.4646	-8.671	-12.007	-11.995	15.331	0.001
C2A	C3A	467.51	-905.2	1.5123	1.23988	1.095	-5.456	-5.453	12.004	0.0006
C3A	H3C	433.38	-1102.35	0.9906	1.46398	-8.65	-11.991	-11.991	15.332	0
C3A	H3D	434.69	-1105.47	0.99	1.46642	-8.668	-12	-11.998	15.33	0.0002
C5A	H5C	434.61	-1105.03	0.9903	1.46602	-8.657	-12.001	-11.995	15.338	0.0005
C5A	H5D	434.69	-1106.58	0.9895	1.46752	-8.709	-12.029	-12.025	15.345	0.0004
C5A	C6A	478.81	-935.13	1.4998	1.26659	0.826	-5.6	-5.596	12.021	0.0007
C6A	H6C	433.38	-1102.15	0.9908	1.46378	-8.642	-11.99	-11.978	15.326	0.001
C6A	H6D	433.9	-1104.01	0.9902	1.46537	-8.673	-12.01	-11.992	15.329	0.0015
C9A	H9A	455.25	-1213.2	0.9498	1.56095	-11.114	-13.248	-13.195	15.329	0.0041
C9A	C10A	577.64	-1227.07	1.3865	1.51553	-2.635	-7.05	-7.024	11.438	0.0037
C10A	H10A	456.03	-1214.72	0.9502	1.56202	-11.113	-13.3	-13.162	15.35	0.0105
C10A	C11A	611.01	-1330.15	1.3536	1.59778	-3.97	-7.556	-7.386	10.972	0.023

C11A	H11A	455.34	-1213	0.9501	1.56072	-11.1	-13.262	-13.171	15.334	0.0069
O1	H1O	316.1	-2111.78	0.8298	2.35338	-54.323	-50.113	-50.057	45.848	0.0011
O1	H1P	324.6	-2103.99	0.8316	2.34467	-53.412	-49.568	-49.53	45.685	0.0008
O2	H2O	392.4	-2028.83	0.8473	2.26475	-45.675	-44.987	-44.905	44.217	0.0018
O2	H2P	410.42	-2004.92	0.8524	2.24025	-43.473	-43.617	-43.611	43.755	0.0002
S3	H5A	11.12	-9	3.0417	0.05233	0.486	-0.123	-0.079	0.688	0.5485
S4	N17A	10.13	-7.67	3.4695	0.04433	0.462	-0.09	-0.043	0.595	1.1052
S4	C7	9.38	-6.88	3.6142	0.03995	0.436	-0.055	-0.036	0.527	0.5395
C18	N8	12.64	-9.16	3.2365	0.04669	0.592	-0.083	-0.028	0.703	2.0193
N17	H9	11.63	-8.68	2.9299	0.04698	0.535	-0.073	-0.036	0.644	1.0209
C20	N8	9.29	-6.43	3.445	0.0353	0.446	-0.064	-0.004	0.514	13.3954
S2A	H1A	33.19	-35.07	2.4452	0.14358	1.149	-0.445	-0.442	2.036	0.0069
S3A	H12	41.6	-46.3	2.3493	0.17424	1.354	-0.552	-0.544	2.45	0.0154
S3A	O1	12.38	-9.55	3.4734	0.05164	0.559	-0.108	-0.048	0.714	1.27