

SUPPLEMENTARY MATERIAL

Synthesis and Structural Characterization of a Series of Group 11 2,2-Dialkyl-1,3-dicyclohexylguanidinate Clusters

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Figure S1. Thermal ellipsoid plot of **2**. Ellipsoids are drawn at the 30 % level. H atoms have been omitted for clarity. The additional “A” letters in the atom labels indicate that these atoms are at $(-x+1, -y, -z)$. Selected inter-atomic distances (Å) and angles ($^{\circ}$): Li(1)-O(1) 1.928(7), Li(1)-N(2) 1.991(7), Li(1)-N(1A) 2.050(7), Li(1)-N(1) 2.283(8), O(1)-Li(1)-N(2) 116.10(4), O(1)-Li(1)-N(1A) 110.70(3), N(2)-Li(1)-N(1A) 129.00(4), O(1)-Li(1)-N(1) 118.80(3), N(2)-Li(1)-N(1) 64.20(2), N(1A)-Li(1)-N(1) 109.00(3).

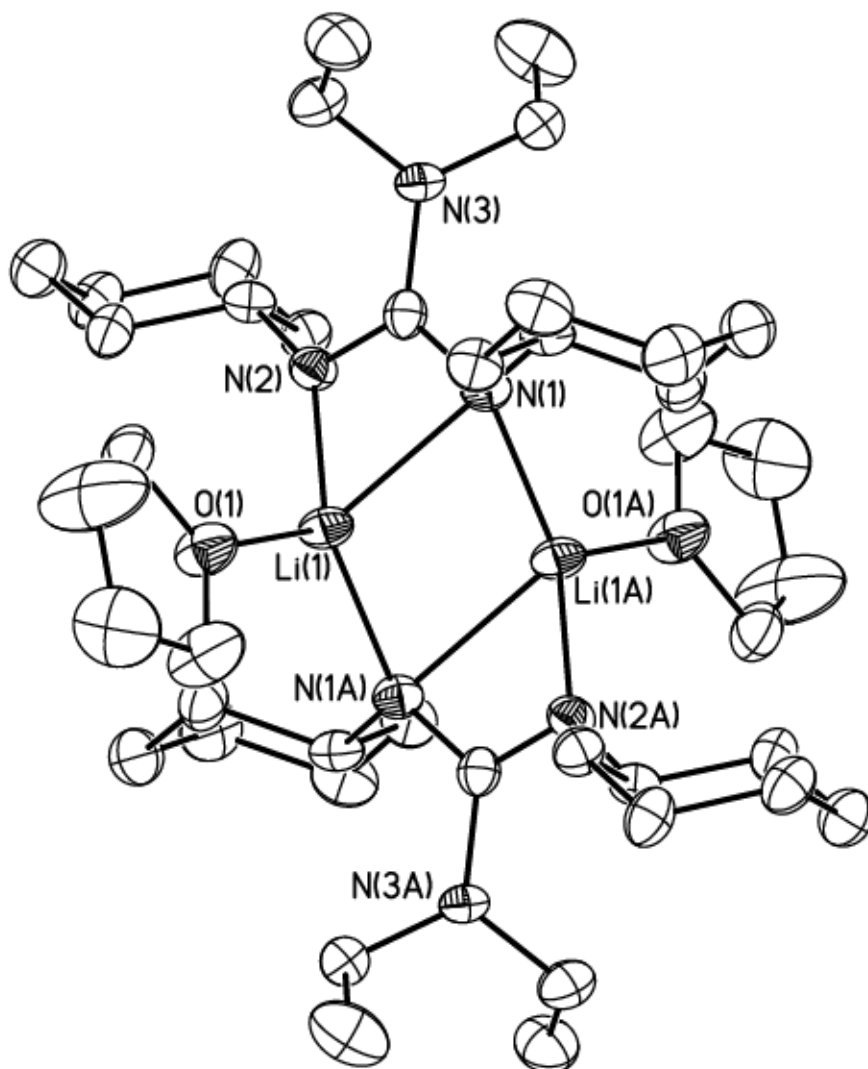


Fig. S2 Thermal ellipsoid plot of **3**. Ellipsoids are drawn at the 30 % level. H atoms have been omitted for clarity. Selected inter-atomic distances (Å) and angles (°): Cu(1)-N(3) 1.877(2), Cu(1)-N(5) 1.882(2), Cu(2)-N(2) 1.875(2), Cu(2)-N(6) 1.876(2), N(3)-Cu(1)-N(5) 170.39(9), N(2)-Cu(2)-N(6) 170.26(9).

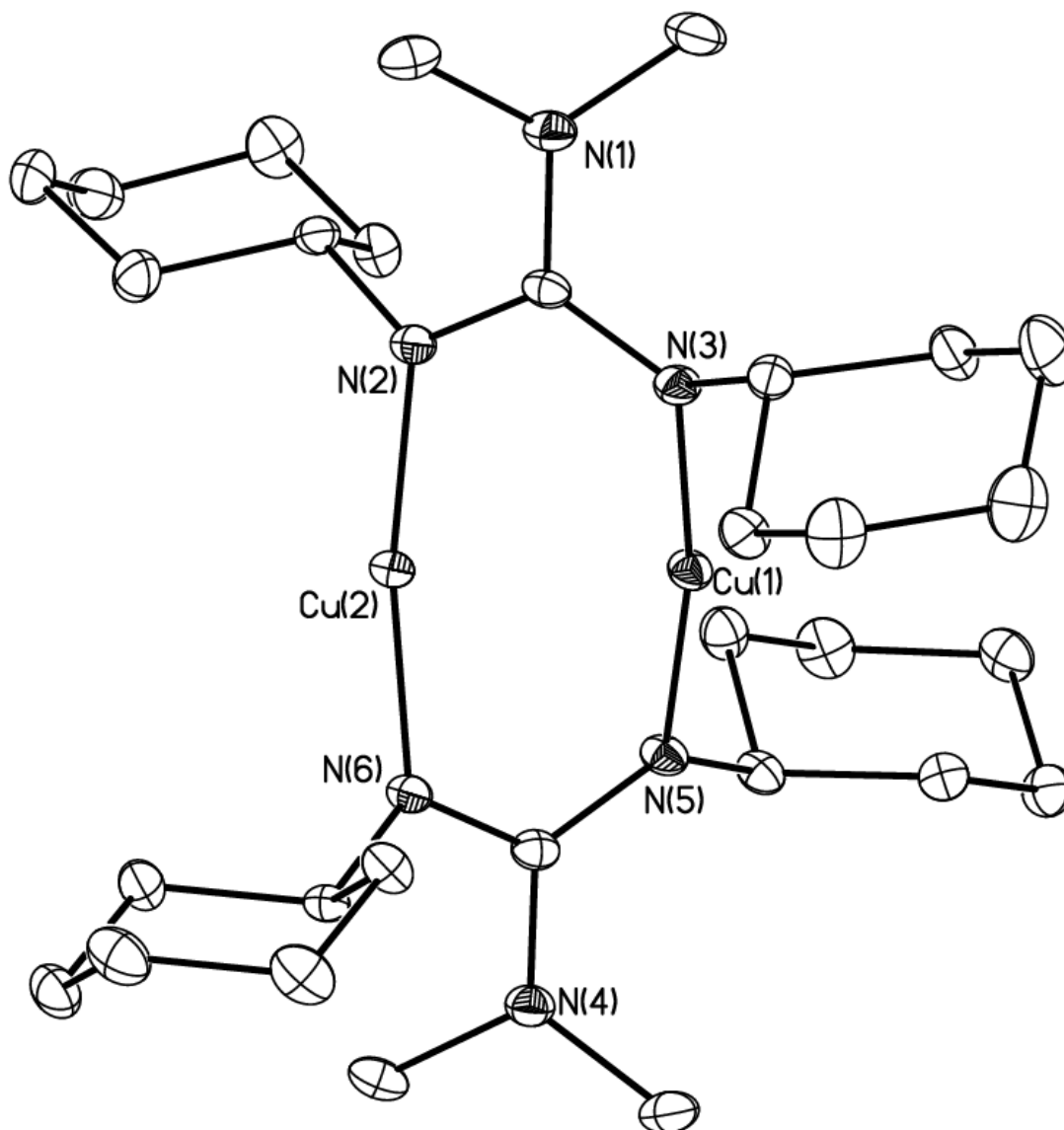


Fig.S3. Thermal ellipsoid plot of **6**. Ellipsoids are drawn at the 30 % level. H atoms have been omitted for clarity. The additional “A” letters in the atom labels indicate that these atoms are at $(-x+1,-y,-z)$. Selected inter-atomic distances (Å) and angles ($^{\circ}$): Ag(1)-N(6) 2.099(6), Ag(1)-N(7) 2.101(6), Ag(2)-N(9) 2.075(6), Ag(2)-N(2) 2.076(6), Ag(3)-N(4) 2.102(6), Ag(3)-N(3) 2.107(6), N(6)-Ag(1)-N(7) 163.4(2), N(9)-Ag(2)-N(2) 169.2(2), N(4)-Ag(3)-N(3) 162.2(2).

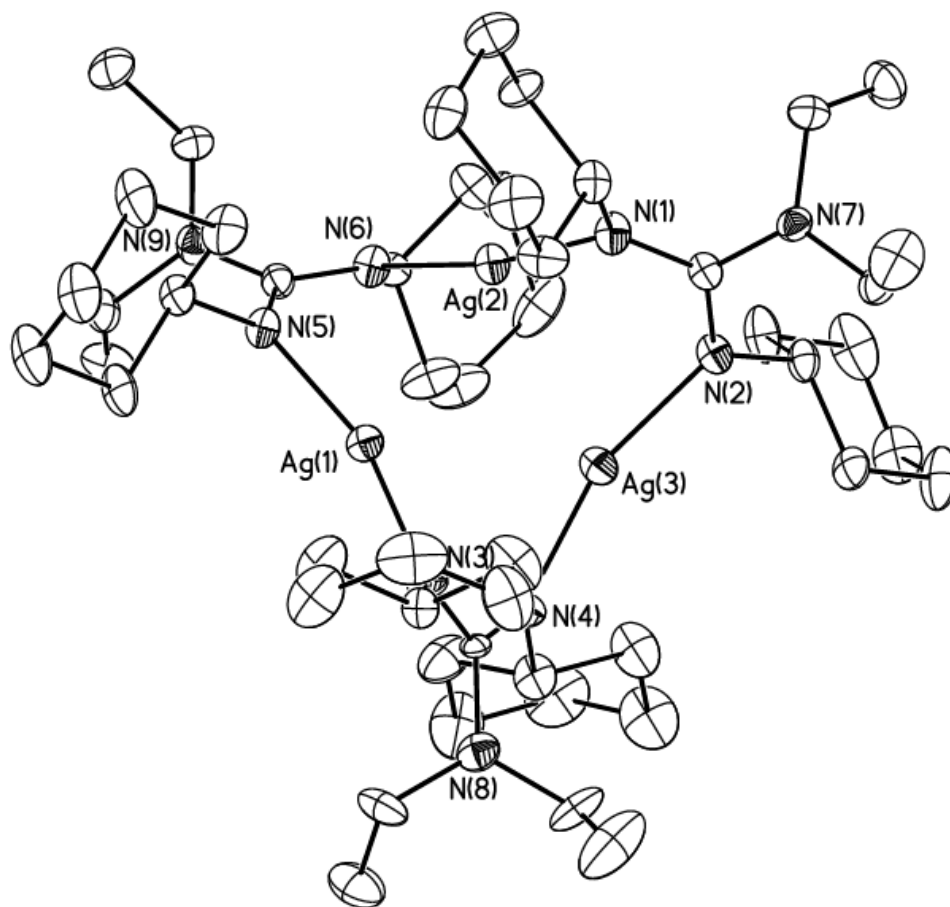


Fig.S4. Thermal ellipsoid plot of **8**. Ellipsoids are drawn at the 30 % level. H atoms have been omitted for clarity. Selected inter-atomic distances (Å) and angles (°): Au(1)-N(1) 2.029(13), Au(1)-Au(1A) 2.6613(14), N(1)-Au(1)-N(1) 165.9(8).

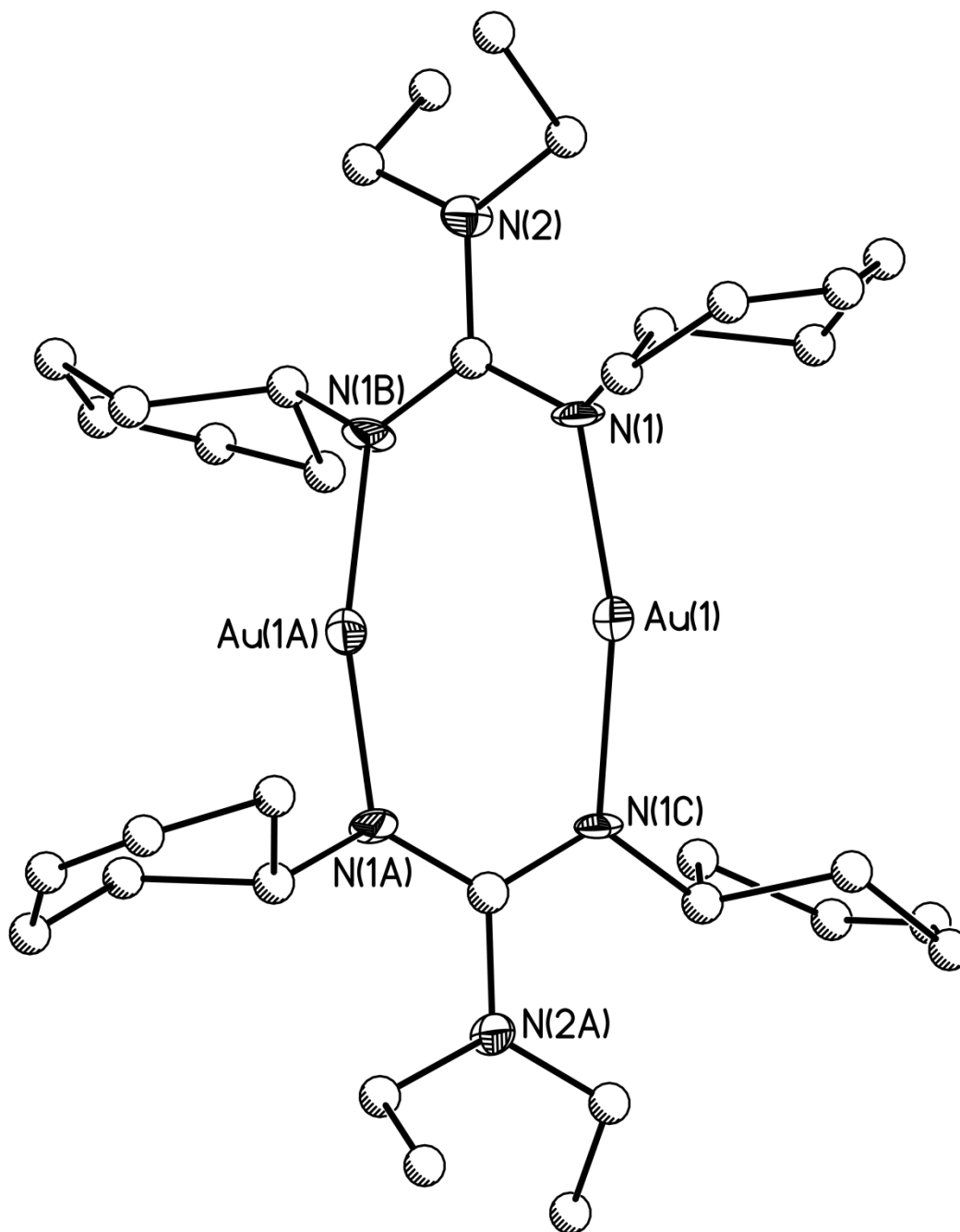
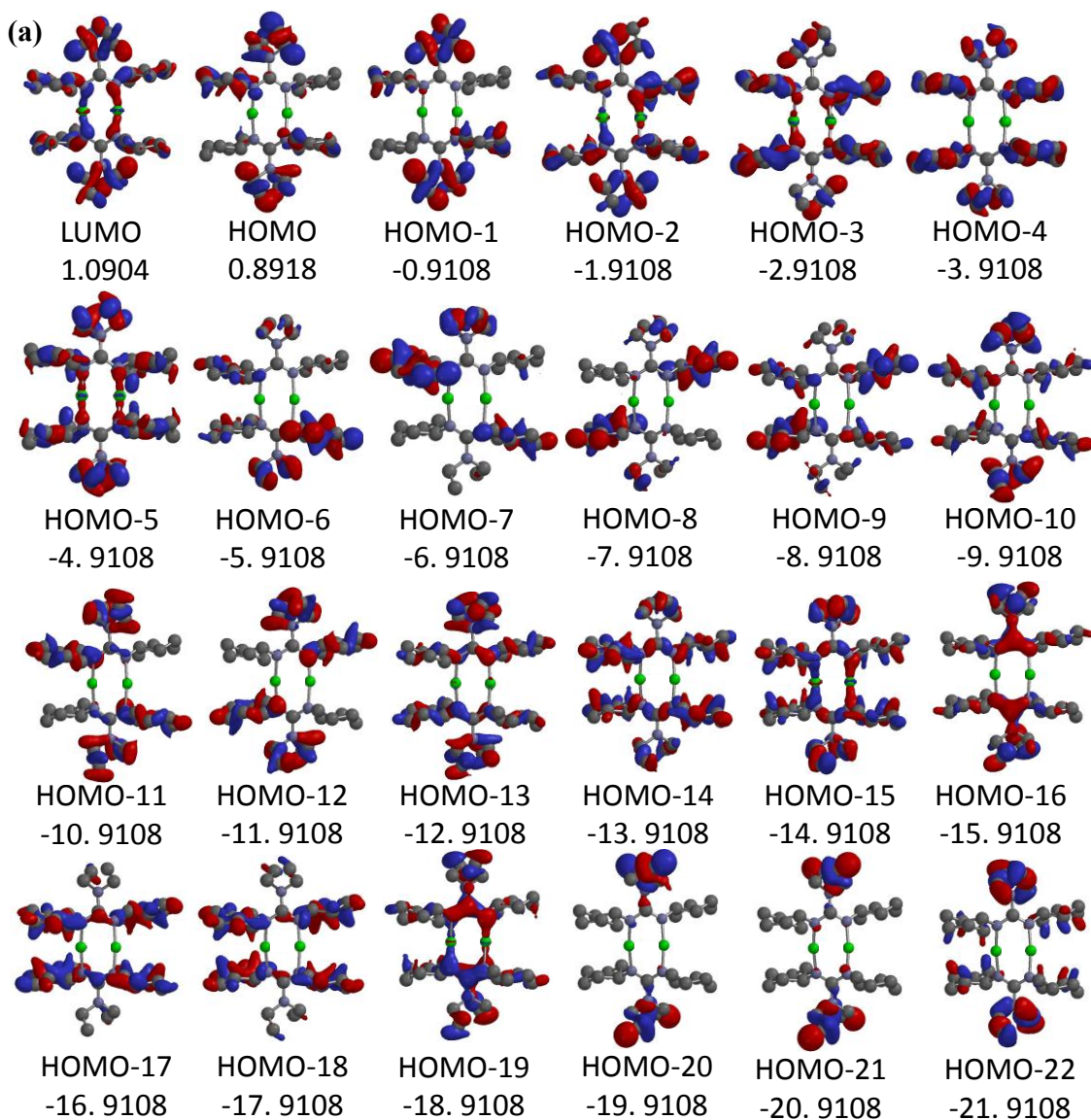
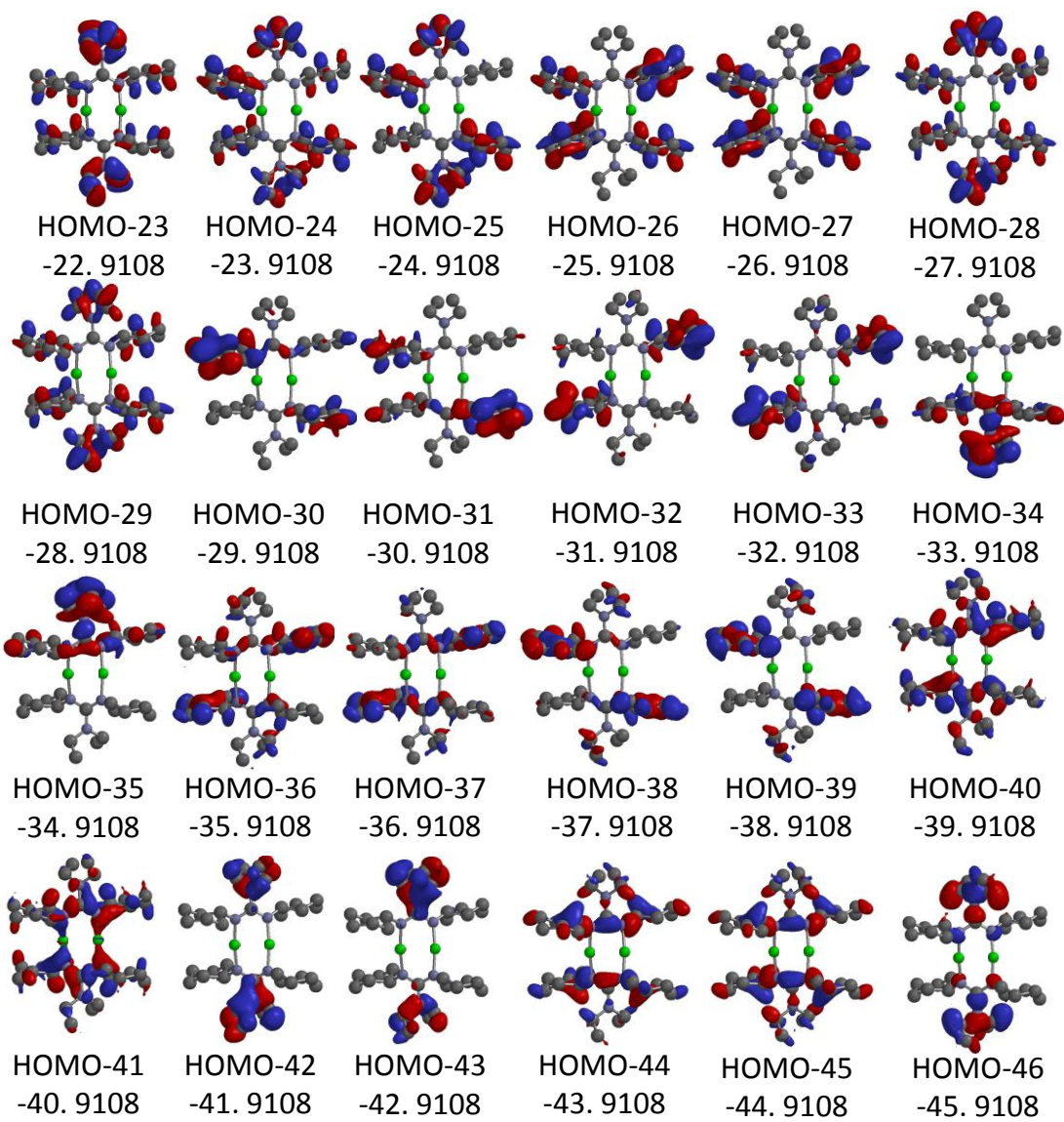
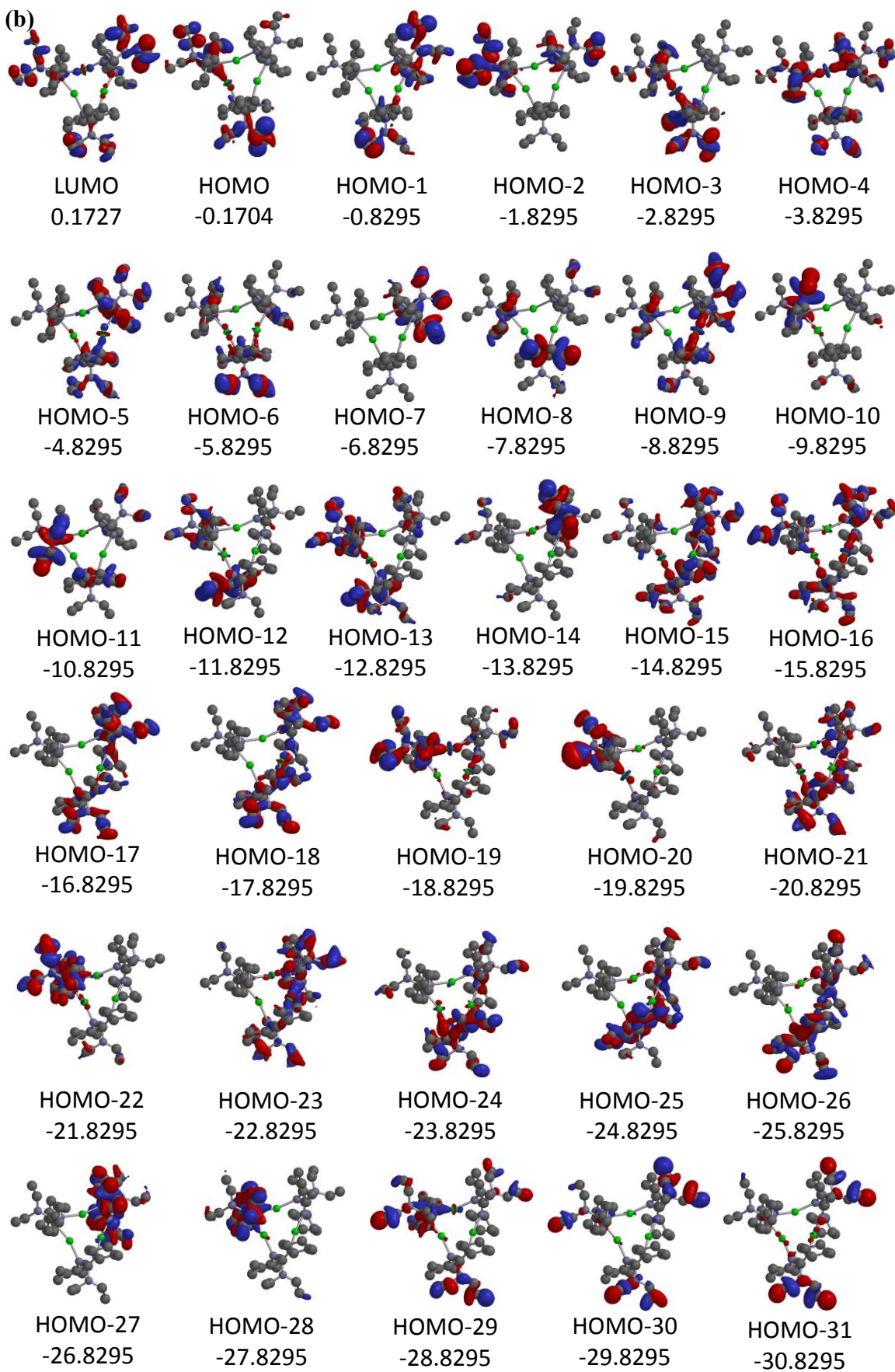
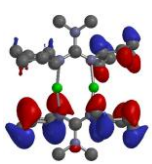


Figure S4. Molecular orbitals of (a) **4** and (b) **6** calculated with B3LYP/LANL2DZ level of theory. (isocontour value of 0.032 au; eigenvalues in eV).

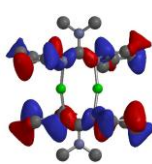




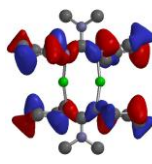




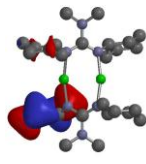
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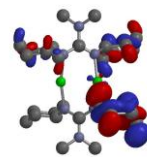
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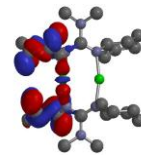
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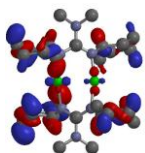
HOMO-50
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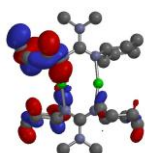
LUMO+1
1.2470



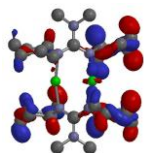
LUMO+2
2.2470



LUMO+3
3.2470



LUMO+4
4.2470



LUMO+5
5.2470

Table S1. Cartesian coordinates for (a) **4** and (b) **6**

(a)

	X	Y	Z		X	Y	Z		X	Y	Z
Cu	0.0763261	-1.2167558	0.0425946	C	-2.5503699	1.9068559	-1.2574121	H	0.6757912	2.0356780	2.6365616
N	-1.7646921	-1.2211723	0.3926078	H	-3.5082841	1.6372225	-1.3564028	H	1.9050503	1.1061724	3.0695603
N	-3.8913075	-0.2653816	0.0476154	C	-2.4987951	3.3528392	-0.7534249	C	2.4966897	0.1549683	0.0485655
N	-1.9000559	0.9895921	-0.3024095	H	-2.9789012	3.4170098	0.1095776	C	4.5368511	1.3432415	-0.6634590
C	-2.3104280	-2.2161103	1.3426197	H	-1.5552236	3.6125093	-0.5984340	H	5.2941430	1.6798812	-0.1234676
H	-3.2988990	-2.0924852	1.4196258	C	-3.1301433	4.3173707	-1.7604280	H	3.8926290	2.0844443	-0.7794606
C	-2.0153992	-3.6413550	0.8716299	H	-4.0948192	4.1138757	-1.8454192	C	5.0529926	0.9073260	-2.0384584
H	-1.0448005	-3.7333327	0.6986237	H	-3.0420772	5.2434237	-1.4234366	H	5.8400276	0.3353993	-1.9254594
H	-2.4928297	-3.8072895	0.0196351	C	-2.4810191	4.2199454	-3.1164312	H	5.2996065	1.7013770	-2.5604667
C	-2.4444193	-4.6977213	1.8996414	H	-1.5404137	4.5225239	-3.0544407	H	4.3508879	0.4118555	-2.5094490
H	-3.4279612	-4.6764370	2.0056483	H	-2.9532024	4.8140475	-3.7514326	C	4.7430762	-0.8019119	0.5715570
H	-2.1884529	-5.5965250	1.5756473	C	-2.5195242	2.7898736	-3.6374187	H	5.2491590	-1.2041661	-0.1784429
C	-1.7819665	-4.4340023	3.2406337	H	-2.0410107	2.7433513	-4.5014213	H	4.1683539	-1.5083378	0.9605669
H	-2.1031991	-5.0962460	3.9016413	H	-3.4601578	2.5227625	-3.7934095	C	5.7078096	-0.3371333	1.6115456
H	-0.8017707	-4.5393924	3.1506276	C	-1.8678333	1.8064959	-2.6344155	H	6.3085549	0.3333371	1.2245357
C	-2.0936858	-3.0454511	3.7326241	H	-1.9492170	0.8798560	-2.9774070	H	6.2329018	-1.1006440	1.9325481
H	-1.6278081	-2.8883784	4.5926190	H	-0.9053609	2.0155717	-2.5414243	H	5.2154350	0.0576319	2.3605455
H	-3.0669274	-2.9631179	3.8936303	Cu	-0.0771656	1.2169319	0.0425752	C	2.5508089	-1.9072646	-1.2574169
C	-1.6612127	-2.0059984	2.7306126	N	1.7647878	1.2217216	0.3925616	H	3.5087217	-1.6376329	-1.3564261
H	-0.6756629	-2.0350908	2.6366057	N	3.8913982	0.2659251	0.0475544	C	2.4979441	-3.3526765	-0.7534046
H	-1.9045486	-1.1065081	3.0696066	N	1.9001415	-0.9890546	-0.3024204	H	2.9789928	-3.4164653	0.1095921
C	-2.4965990	-0.1544249	0.0486043	C	2.3105375	2.2166757	1.3425488	H	1.5553049	-3.6119767	-0.5983956
C	-4.5364035	-1.3436401	-0.6633705	H	3.2993769	2.0921217	1.4195426	C	3.1305751	-4.3177878	-1.7604005
H	-5.2946177	-1.6806379	-0.1233624	C	2.0158691	3.6409822	0.8715392	H	4.0948824	-4.1133642	-1.8454092
H	-3.8931132	-2.0852122	-0.7793689	H	1.0452678	3.7329571	0.6985455	H	3.0425138	-5.2438352	-1.4233922
C	-5.0525649	-0.9077478	-2.0383698	H	2.4932872	3.8069024	0.0195347	C	2.4810638	-4.2194553	-3.1163960
H	-5.8399656	-0.3348891	-1.9253690	C	2.4436068	4.6979288	1.8995266	H	1.5395293	-4.5224000	-3.0543866
H	-5.2995536	-1.7008776	-2.5603611	H	3.4284476	4.6760834	2.0055196	H	2.9536052	-4.8144982	-3.7513941
H	-4.3508343	-0.4113552	-2.5093789	H	2.1885658	5.5970943	1.5755211	C	2.5189985	-2.7906897	-3.6374081
C	-4.7429779	0.8024642	0.5716123	C	1.7821036	4.4345997	3.2405330	H	2.0404725	-2.7441819	-4.5014046
H	-5.2490715	1.2047057	-0.1783871	H	2.1033457	5.0968545	3.9015248	H	3.4605600	-2.5232140	-3.7934171
H	-4.1688128	1.5075993	0.9606020	H	0.8022737	4.5390581	3.1505393	C	1.8669550	-1.8063650	-2.6344121
C	-5.7086263	0.3373359	1.6116227	C	2.0932671	3.0447594	3.7325423	H	1.9496311	-0.8802937	-2.9774204
H	-6.3084471	-0.3327737	1.2246329	H	1.6283320	2.8880685	4.5925466	H	0.9044839	-2.0154391	-2.5414034
H	-6.2337139	1.1008520	1.9326199	H	3.0674412	2.9627962	3.8935358				
H	-5.2162409	-0.0574166	2.3606221	C	1.6617096	2.0056570	2.7305547				

(b)

	X	Y	Z		X	Y	Z		X	Y	Z
Ag	-1.4805713	-0.9435588	0.3308496	H	7.1866059	0.8592339	-0.9515305	H	-3.2461689	-2.0645885	2.8664247
Ag	-0.2795186	1.2183027	-1.3459763	H	5.9662943	-0.1388496	-0.6685511	H	-3.1823130	-0.4984807	2.5315034
Ag	1.5232831	0.0172409	0.6643583	C	5.4293579	1.4972074	-1.7411376	C	-1.4761300	-1.1923024	3.4427711
N	1.9441621	4.3079566	0.5319345	H	5.5654712	1.0526515	-2.6149197	H	-1.2665088	-1.8964540	4.1194613
N	0.2016354	2.8917408	-0.2162061	H	5.7254193	2.4375192	-1.8229949	C	-4.4168508	0.7075751	-0.9135304
N	2.2427135	1.9681610	0.3217437	C	3.9333872	1.4575051	-1.3680767	H	-4.0960101	1.3566635	-1.5882078
N	1.3366194	-1.9507300	1.3788716	H	3.4101122	1.9525082	-2.0461586	H	-3.9550967	0.9020053	-0.0585461
N	0.6368064	-3.0307878	3.3662056	H	3.6199570	0.5189181	-1.3644582	C	-5.9407189	0.8754440	-0.7237339
N	-0.7722806	-1.5062020	2.2230797	C	3.6256250	-2.4250087	0.7153590	H	-6.1299520	1.7801355	-0.3683339
N	-2.5858563	-0.8290507	-1.4537049	H	3.9738162	-1.9108631	1.4865731	H	-6.3913259	0.7904354	-1.6000871
N	-2.6364670	-1.3225092	-3.7696458	H	3.5137524	-1.8000026	-0.0433017	C	-6.4897492	-0.1496774	0.2149784
N	-0.8118355	-0.1967606	-2.7669401	C	4.6440438	-3.5353867	0.3293754	H	-7.4711743	-0.0399256	0.2851812
C	-1.8111735	4.1187016	-0.8895580	H	5.5056361	-3.1206172	0.0731663	H	-6.0995964	-0.0131589	1.1146558
H	-2.1655246	3.2682337	-1.2530614	H	4.8058748	-4.1237457	1.1093231	C	-6.1720905	-1.5588335	-0.2633487
H	-1.3144782	4.5738285	-1.6136218	C	4.1266174	-4.3448407	-0.8034217	H	-6.6106592	-1.7196508	-1.1358145
C	-2.9790166	4.9981300	-0.4573186	H	4.7776158	-5.0557913	-1.0247098	H	-6.5246191	-2.2175800	0.3861971
H	-2.6380253	5.8881729	-0.1877159	H	4.0218671	-3.7660209	-1.6009423	C	-4.6517126	-1.7409157	-0.4090226
H	-3.5974375	5.1236223	-1.2204827	C	2.8140703	-4.9586743	-0.4610502	H	-4.2200939	-1.6515652	0.4785819
C	-3.7143573	4.3716196	0.6897745	H	2.9303101	-5.5891439	0.2953574	H	-4.4590221	-2.6501479	-0.7520361
H	-4.4390866	4.9774579	0.9844190	H	2.4735903	-5.4698593	-1.2364800	C	-4.0676513	-0.7029101	-1.3652227
H	-4.1266394	3.5228096	0.3906004	C	1.7879742	-3.8687492	-0.0709757	H	-4.4563620	-0.8527366	-2.2742178
C	-2.7977570	4.1024950	1.8346304	H	1.6155136	-3.2858851	-0.8528771	C	-1.9984634	-0.7777929	-2.6368476
H	-3.3012399	3.6554047	2.5602248	H	0.9344307	-4.2970585	0.1861773	C	-2.6821850	-0.6265039	-5.0147460
H	-2.4484527	4.9585249	2.1864037	C	2.2903834	-3.0299142	1.0742002	H	-2.3291143	-1.2167045	-5.7277456
C	-1.6084350	3.1976183	1.3934446	H	2.3983126	-3.6094770	1.8805719	H	-2.0920581	0.1674661	-4.9613130
H	-0.9929755	3.0666222	2.1580011	C	0.3948895	-2.1608329	2.3016391	C	-4.0962258	-0.1732546	-5.3959605
H	-1.9524715	2.3099846	1.1218614	C	1.8673379	-2.9197153	4.1434842	H	-4.6741210	-0.9586281	-5.4971269
C	-0.8520569	3.8097622	0.2465154	H	2.3132152	-3.8042968	4.1404792	H	-4.0645163	0.3212739	-6.2407535
H	-0.4291880	4.6610975	0.5552048	H	2.4684295	-2.2858036	3.6773492	H	-4.4546306	0.4058437	-4.6907895
C	1.4570554	3.0263104	0.2070326	C	1.7375866	-2.4938130	5.4942573	C	-2.2569981	-3.7083977	-4.3001874
C	1.8118280	5.3978133	-0.4114017	H	1.4100281	-1.5703758	5.5161014	H	-1.9437349	-3.4198920	-5.1817092
H	1.5289732	6.2118661	0.0746335	H	2.6113119	-2.5412374	5.9376232	H	-2.7356078	-4.5593811	-4.3848997
H	1.1007396	5.1743512	-1.0632445	H	1.1029893	-3.0763419	5.9608088	H	-1.4912392	-3.8224884	-3.7007196
C	3.0844315	5.6963586	-1.1642589	C	0.2200048	-5.4630863	3.4264088	C	-3.1937787	-2.6585213	-3.7290830
H	3.7930268	5.9231764	-0.5267173	H	0.3648515	-5.5653644	2.4647889	H	-4.0407214	-2.6709324	-4.2399648
H	2.9367283	6.4514057	-1.7702256	H	-0.4287884	-6.1319757	3.7339938	H	-3.4035906	-2.8914968	-2.7901227
H	2.0942501	6.4412215	2.2408446	H	-1.2274842	0.8485342	3.3254802	C	1.1080184	-1.6455987	-3.0153164
H	2.5770595	5.5753325	3.4984089	H	-0.0592671	0.1230676	4.1503884	H	0.5948946	-2.4128656	-2.6558022
H	1.1510405	5.2893655	2.8306632	C	-1.7751780	0.4610825	5.3195939	H	1.5073906	-1.1623619	-2.2488092
C	3.6890255	2.0805329	0.0139681	H	-1.5205908	-0.2024218	6.0084019	C	2.2302622	-2.1726287	-3.9111372
H	3.9355256	3.0495790	-0.0223701	H	-1.5011990	1.3571498	5.6399810	H	2.8591410	-2.7117348	-3.3687968
C	4.5340936	1.4110643	1.0509230	C	-3.2614469	0.4339025	5.1178663	H	1.8472927	-2.7609435	-4.6085246
H	4.2464163	0.4696041	1.1518169	H	-3.5238437	1.1737707	4.5167939	C	2.9781386	-1.0390278	-4.5676841
H	4.4118927	1.8657907	1.9212401	H	-3.7116393	0.5753329	5.9891868	H	3.4675453	-0.5235175	-3.8771254
C	6.0240823	1.4498627	0.6586944	C	-3.7243626	-0.8698275	4.5294610	H	3.6419531	-1.4069077	-5.2032522
H	6.3369304	2.3899560	0.6360921	H	-4.6957376	-0.8216970	4.3451511	C	2.0445762	-0.1373336	-5.2936232
H	6.5578783	0.9634779	1.3336083	H	-3.5702130	-1.5987721	5.1804954	H	1.6374252	-0.6312902	-6.0501019
C	6.2277710	0.8142972	-0.7078743	C	-2.9596760	-1.1822181	3.2109944	H	2.5518450	0.6253855	-5.6663297