

Supporting information

Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study

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Table S1: The interaction energies, ΔE (kcal mol⁻¹) of rh-Ag₄ clusters over coronene substrate calculated at two different positions.

Method/basis set	Ag ₄ (Energy in a.u)	Coronene (Energy in a.u)	Ag ₄ -coronene Str;3 (Energy in a.u)	ΔE (Kcal/mol)	ΔE (Kcal/mol) (literature)
M062X/LANL2DZ	-582.7540905	-921.4263281	-1504.2045968	-15.172	13.68
	Ag ₄ (Energy in a.u)	Coronene (Energy in a.u)	Ag ₄ -coronene Str;4 (Energy in a.u)	ΔE (Kcal/mol)	ΔE (Kcal/mol) (literature)
-do-	-582.7540905	-921.4263281	-1504.2046097	-15.180	13.32
Pbe/lanl2dz	-583.0252623	-920.6241584	-1503.6688113	-12.167	-do-

Table S2. INTERACTION ENERGIES (ΔE) OF Ag₂-coronene (singlet) (M062X/LANL2DZ)

S No	Ag ₂ (Energy in a.u)	Coronene (Energy in a.u)	Ag ₂ -coronene complex (Energy in a.u)	ΔE (kcal/mol)
21	-291.3616933	-921.4261564	-1212.8006997	-8.06349
22	-291.3616933	-921.4261564	-1212.8010849	-8.30521
23	-291.3616933	-921.4261564	-1212.8008941	-8.18548
24 -A	-291.3616933	-921.4261564	-1212.8010878	-8.30703
25	-291.3616933	-921.4261564	-1212.8009096	-8.19521
26	-291.3616933	-921.4261564	-1212.8008061	-8.13026
27	-291.3616933	-921.4261564	-1212.8007078	-8.06857
28-B	-291.3616933	-921.4261564	-1212.8019777	-8.86545

Table S3. INTERACTION ENERGIES OF Ag₃-coronene(doublet) (M062X/LANL2DZ)

S No	Ag ₃ (Energy in a.u)	Coronene (Energy in a.u)	Ag ₃ -coronene complex (Energy in a.u)	ΔE (kcal/mol)
311-A	-437.0435799	-921.4261564	-1358.4905202	-13.04209469
312-B	-437.0435799	-921.4261564	-1358.4834389	-8.5985116747
321	-437.0435941	-921.4261564	-1358.4907615	-13.18460210
322	-437.0435941	-921.4261564	-1358.4905236	-13.03531759

Table S4. INTERACTION ENERGIES (ΔE) OF Ag₄-coronene (singlet) at M062X/LANL2DZ

S No	Ag4 (Energy in a.u)	Coronene (Energy in a.u)	Ag4-coronene complex (Energy in a.u)	ΔE (kcal/mol)
411	-582.7540903	-921.4261564	-1504.2045663	-15.2608
411p	-582.7540903	-921.4261564	-1504.2041878	-15.0233
412	-582.7540903	-921.4261564	-1504.2045976	-15.2804
413	-582.7540903	-921.4261564	-1504.2045959	-15.2793
421	-582.748795	-921.4261564	-1504.1996498	-15.4985
422	-582.748795	-921.4261564	-1504.1995335	-15.4255
423	-582.748795	-921.4261564	-1504.1934127	-11.5846
431	-582.7305018	-921.4261564	-1504.2031389	-29.1671
432	-582.7305018	-921.4261564	-1504.2045633	-30.0609

Table S5. INTERACTION ENERGIES (ΔE) OF Ag5-corrone (doublet) M06-2X/LANL2DZ

S No	Ag5 (Energy in a.u)	Coronene (Energy in a.u)	Ag5-coronene complex (Energy in a.u)	ΔE (kcal/mol)
511-D	-728.4631329	-921.4261564	-1649.9187448	-18.4836
512-A	-728.4631329	-921.4261564	-1649.9188844	-18.5712
513-E	-728.4631329	-921.4261564	-1649.9186418	-18.4189
514-B	-728.4631329	-921.4261564	-1649.9114369	-13.8978
521	-728.4631329	-921.4261564	-1649.9186396	-28.2632
522-F	-728.4631329	-921.4261564	-1649.9186406	-28.2638
523-C	-728.4631329	-921.4261564	-1649.9085978	-21.9618
524	-728.4631329	-921.4261564	-1649.9186356	-28.2606
525	-728.4631329	-921.4261564	-1649.9186442	-28.2660
531-G	-728.4631329	-921.4261564	-1649.9186420	-18.3311
532-H	-728.4631329	-921.4261564	-1649.9186438	-18.4202
533-I	-728.4631329	-921.4261564	-1649.9186400	-18.4179

Table S6. INTERACTION ENERGIES (ΔE) OF Ag6-corrone (singlet) (M062X/LANL2DZ)

S No	Ag6 (Energy in a.u)	Coronene (Energy in a.u)	Ag6-coronene Complex (Energy in a.u)	ΔE kcal/mol
611-C	-874.188128	-921.4261564	-1795.6449995	-19.27401704
612-D	-874.188128	-921.4261564	-1795.6371505	-14.34869498
621-A	-874.1819697	-921.4261564	-1795.6423442	-21.47218282
622-E	-874.1819697	-921.4261564	-1795.6423368	-21.46753925
631-F	-874.1819697	-921.4261564	-1795.642361	-21.48272498
632	-874.1819697	-921.4261564	-1795.6423353	-21.46659799
633-B	-874.1819697	-921.4261564	-1795.635887	-17.42022848
641-G	-874.188128	-921.4261564	-1795.6450548	-19.30871832
642-H	-874.188128	-921.4261564	-1795.6452002	-19.3999582
643-I	-874.188128	-921.4261564	-1795.6445957	-19.02062871

Table S7. INTERACTION ENERGIES (ΔE) OF Ag7-corrone (doublet) (M062X/LANL2DZ)

S No	Ag7 (Energy in a.u)	Coronene (Energy in a.u)	Ag7-coronene complex (Energy in a.u)	ΔE (kcal/mol)
711	-1019.8955838	-921.4261564	-1941.3470776	-15.89945920
712	-1019.8955838	-921.4261564	-1941.3475731	-16.21039016
713-A	-1019.8955838	-921.4261564	-1941.3477727	-16.33564105
721-B	-1019.8745608	-921.4261564	-1941.339314	-24.21985866
722	-1019.8745608	-921.4261564	-1941.3384688	-23.689487764

Table S8. INTERACTION ENERGIES (ΔE) OF Ag8-corrone (singlet) (M062X/LANL2DZ)

S No	Ag8 (Energy in a.u)	Coronene (Energy in a.u)	Ag8-coronene complex (Energy in a.u)	ΔE (kcal/mol)
811-A	-1165.5903002	-921.4261564	-2087.0564536	-25.09837748
812-B	-1165.5903002	-921.4261564	-2087.0420193	-16.0483709
821	-1165.6199712	-921.4261564	-2087.0719664	-16.21409246
822	-1165.6199712	-921.4261564	-2087.0722413	-16.38659483
823-C	-1165.6199712	-921.4261564	-2087.0740351	-17.51222137

Table S9. INTERACTION ENERGIES (ΔE) OF Ag9-corrone (doublet) (M062X/LANL2DZ)

S No	Ag9 (Energy in a.u)	Coronene (Energy in a.u)	Ag9-coronene complex (Energy in a.u)	ΔE (kcal/mol)
911	-1311.3161468	-921.4261564	-2232.7695453	-17.09467655

912-C	-1311.3161468	-921.4261564	-2232.7739416	-19.85339656
921-D	-1311.3143956	-921.4261564	-2232.7663783	-16.2062486
931-E	-1311.2903259	-921.4261564	-2232.7584634	-26.34353907
932	-1311.2903259	-921.4261564	-2232.7378415	-13.40310091
941-B	-1311.2862397	-921.4261564	-2232.7551763	-26.84498191
942	-1311.2862397	-921.4261564	-2232.7417886	-18.44407297
951-A	-1311.2977896	-921.4261564	-2232.7706414	-29.30180710
952	-1311.2977896	-921.4261564	-2232.7666419	-26.79208286
953	-1311.2977896	-921.4261564	-2232.7641436	-25.22437587

Table S10. INTERACTION ENERGIES (ΔE) OF Ag10-corrone(singlet) (M062X/LANL2DZ)

S No	Ag10 (Energy in a.u)	Coronene (Energy in a.u)	Ag10-coronene complex (Energy in a.u)	ΔE (kcal/mol)
1011-A	-1457.0151382	-921.4261564	-2378.4900614	-30.60163028
1012-B	-1457.0151382	-921.4261564	-2378.4872999	-28.8687628

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Table S11. INTERACTION ENERGIES (ΔE) OF Ag2-corrone(triplet) (M062X/LANL2DZ)

S No	Ag2 (Energy in a.u)	Coronene (Energy in a.u)	Ag2-coronene complex (Energy in a.u)	ΔE (kcal/mol)
21t	-182800.3914912966	-578203.6666894858	-761017.6754437846	-13.6172
22t	-182800.3914912966	-578203.6666894858	-761017.6754375095	-13.6172
23t	-182800.3914912966	761004.0581807824	-761017.6754186841	-13.6172
24t	-182800.3914912966	761004.0581807824	-761017.6755065356	-13.6173
25t	-182800.3914912966	761004.0581807824	-761017.6753622083	-13.6171
26t	-182800.3914912966	761004.0581807824	-761017.6841096907	-13.6259
27t	-182800.3914912966	761004.0581807824	-761017.6755002603	-13.6173

Table S12. INTERACTION ENERGIES (ΔE) OF Ag3-corrone(quartet) (M062X/LANL2DZ)

S No	Ag3 (Energy in a.u)	Coronene (Energy in a.u)	Ag3-coronene complex (Energy in a.u)	ΔE (kcal/mol)
311q	-274201.5262933027	-578203.6666894858	-852429.6234066634	-24.4304
312q	-274201.5262933027	-578203.6666894858	-852429.6205577702	-24.4275
321q	-274205.71680299874	-578203.6666894858	-852430.0353164495	-20.6518
322q	-274205.71680299874	-578203.6666894858	-852429.922665944	-20.5391

Table S13. INTERACTION ENERGIES (ΔE) OF Ag4-corrone(triplet) (M062X/LANL2DZ)

S No	Ag4 (Energy in a.u)	Coronene (Energy in a.u)	Ag4-coronene complex (Energy in a.u)	ΔE (kcal/mol)
411t	-365672.65027389245	-578203.6666894858	-943894.5021849233	-18.1852215451
412t	-365672.65027389245	-578203.6666894858	-943894.4304166617	-18.1134532835
413t	-365672.65027389245	-578203.6666894858	-943894.4158709914	-18.0989076132
421t	-365663.09322953376	-578203.6666894858	-943870.9908409549	-4.2309219354
422t	-365663.09322953376	-578203.6666894858	-943894.0203203781	-27.2604013586
423t	-365663.09322953376	-578203.6666894858	-943880.388762082	-13.6288430625
431t	-365672.6300417312	-578203.6666894858	-943894.5011997331	-18.2044685161
432t	-365672.6300417312	-578203.6666894858	-943894.3694666638	-18.0727354468

Table S14. INTERACTION ENERGIES (ΔE) OF Ag5-corrone(quartet) (M062X/LANL2DZ)

S No	Ag5 (Energy in a.u)	Coronene (Energy in a.u)	Ag5-coronene complex (Energy in a.u)	ΔE (kcal/mol)
511q	-457078.3237259826	-578203.6666894858	-1035304.5168788838	-22.5264634146
512q	-457078.3237259826	-578203.6666894858	-1035304.7186294632	-22.728213995
513q	-457078.3237259826	-578203.6666894858	-1035304.7348505837	-22.744435115
514q	-457078.3237259826	-578203.6666894858	-1035317.2330953473	-35.242679879
521q	-457073.646826143	-578203.6666894858	-1035318.0104729413	-40.6969573122
522q	-457073.646826143	-578203.6666894858	-1035317.0142639595	-39.70074833
523q	-457073.646826143	-578203.6666894858	-1035317.0135548736	-39.700039244
524q	-457073.646826143	-578203.6666894858	-1035303.5405682282	-26.227052599
525q	-457073.646826143	-578203.6666894858	-1035303.2571472875	-25.943631658
531q	-457096.3063297301	-578203.6666894858	-1035317.8489331707	-17.8759139541
532q	-457096.3063297301	-578203.6666894858	-1035317.0087669762	-17.03574776
533q	-457096.3063297301	-578203.6666894858	-1035317.2236764297	-17.250657213

Table S15. INTERACTION ENERGIES (ΔE) OF Ag6-corrone(triplet) (M062X/LANL2DZ)

S No	Ag6 (Energy in a.u)	Coronene (Energy in a.u)	Ag6-coronene complex (Energy in a.u)	ΔE (kcal/mol)
611t	-548538.8525249296	-578203.6666894858	-1126765.3486852257	-22.8294708096
612t	-548538.8525249296	-578203.6666894858	-1126765.3523185058	-22.83310409
621t	-548544.2669341746	-578203.6666894858	-1126765.2369132335	-17.3032895726
622t	-548544.2669341746	-578203.6666894858	-1126782.6326562914	-34.699032631

631t	-548544.2666549328	-578203.6666894858	-1126765.371037114	-17.4376926954
632t	-548544.2666549328	-578203.6666894858	-1126765.1727001865	-17.239355767
633t	-548544.2666549328	-578203.6666894858	-1126767.883917732	-19.950573313
641t	-548557.4858026903	-578203.6666894858	-1126784.2975205712	-23.1450283949
642t	-548557.4858026903	-578203.6666894858	-1126765.1022936204	-3.949801444
643t	-548557.4858026903	-578203.6666894858	-1126765.3528142383	-4.200322062

Table S16. INTERACTION ENERGIES (ΔE) OF Ag7-corrone(quartet) (M062X/LANL2DZ)

S No	Ag7 (Energy in a.u)	Coronene (Energy in a.u)	Ag7-coronene complex (Energy in a.u)	ΔE (kcal/mol)
711q	-639966.7054791375	-578203.6666894858	-1218192.1146197869	-21.7424511627
712q	-639966.7054791375	-578203.6666894858	-1218192.2328425767	-21.860673953
713q	-639966.7054791375	-578203.6666894858	-1218192.2235428859	-21.851374262
721q	-639994.2311394294	-578203.6666894858	-1218176.3669488546	21.5308800612
722q	-639994.2311394294	-578203.6666894858	-1218176.2762674568	21.621561459

Table S17. INTERACTION ENERGIES (ΔE) OF Ag8-corrone(triplet) (M062X/LANL2DZ)

S No	Ag8 (Energy in a.u)	Coronene (Energy in a.u)	Ag8-coronene complex (Energy in a.u)	ΔE (kcal/mol)
811t	-731406.2044223166	-578203.6666894858	-1309635.068435745	-21.4500254615
812t	-731406.2044223166	-578203.6666894858	-1309634.037933369	-24.166821567
821t	-731409.9517207977	-578203.6666894858	-1309639.103453607	-25.485043323
822t	-731409.9517207977	-578203.6666894858	-1309640.2397854603	-26.621375176
823t	-731409.9517207977	-578203.6666894858	-1309639.611334696	-25.992924412

Table S18. INTERACTION ENERGIES (ΔE) OF Ag9-corrone(quartet) (M062X/LANL2DZ)

S No	Ag9 (Energy in a.u)	Coronene (Energy in a.u)	Ag9-coronene complex (Energy in a.u)	ΔE (kcal/mol)
911q	-822841.6529987513	-578203.6666894858	-1401067.2534168463	-21.9337286089
912q	-822841.6529987513	-578203.6666894858	-1401069.2971337116	-23.977445474
921q	-822841.6526787214	-578203.6666894858	-1401063.2104672643	-17.8910990568
931q	-822826.1534576253	-578203.6666894858	-1401057.3779170641	-27.5577699529
932q	-822826.1534576253	-578203.6666894858	-1401064.1186241133	-34.298477002
941q	-822844.5726498525	-578203.6666894858	-1401058.9550178652	-10.7156785267
942q	-822844.5726498525	-578203.6666894858	-1401057.4772894685	-9.23795013
951q	-822831.8511811345	-578203.6666894858	-1401064.6329999254	-29.1151293047
952q	-822831.8511811345	-578203.6666894858	-1401064.630929144	-29.113058524
953q	-822831.8511811345	-578203.6666894858	-1401068.2332352803	-32.71536466

Table S19. INTERACTION ENERGIES (ΔE) OF Ag10-corrone(triplet) (M062X/LANL2DZ)

S No	Ag10 (Energy in a.u)	Coronene (Energy in a.u)	Ag10-coronene complex (Energy in a.u)	ΔE (kcal/mol)
1011t	-914291.6235067114	-578203.6666894858	-1492515.8949789125	-20.6047827148

1012t	-914291.6235067114	-578203.6666894858	-1492519.755254204	-24.465058007
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Table S20. ENERGIES of silver-coronene composite (VARIOUS SPIN MULTIPLICITIES) FOR MOST STABLE Ag_n...Coronene (n=2-10) composites

Ag _n ...Coronene	Ground Spin multiplicity	(Energy in a.u)	First higher spin multiplicity	(Energy in a.u)
Ag2...Coronene	Singlet	-1212.8010878	Triplet	-1212.75882534
Ag3...Coronene	Doublet	-1358.4907615	Quintet	-1358.43367362
Ag4...Coronene	Singlet	-1504.2045976	Triplet	-1504.19157349
Ag5...Coronene	Doublet	-1649.9188844	Quintet	-1649.88420171
Ag6...Coronene	Singlet	-1795.6452002	Triplet	-1795.64500222
Ag7...Coronene	Doublet	-1941.3477727	Quintet	-1941.31281334
Ag8...Coronene	Singlet	-2087.0740351	Triplet	-2087.04448265
Ag9...Coronene	Doublet	-2232.7739416	Quintet	-2232.74425843
Ag10...Coronene	Singlet	-2378.4900614	Triplet	-2378.47537763

Table S21. binding Energy (kcal mol⁻¹) of most stable Ag_n...DBC (n=2-10) composites at M062X.

Silver clusters	Ag _n (n=2-10), Energy (kcal mol ⁻¹)	DBC, Energy (kcal mol ⁻¹)	Ag _n ...DBC composite	Energy (kcal mol ⁻¹)	binding Energy (kcal mol ⁻¹)
Ag ₂	-182832.2306	-1297658.429	Ag ₂ ...DBC	-1480494.229	-3.56
Ag ₃	-274249.033	-1297658.429	Ag ₃ ...DBC	-1571916.526	-9.06
Ag ₄	-365683.7446	-1297658.429	Ag ₄ ...DBC	-1663353.573	-11.39
Ag ₅	-457117.5923	-1297658.429	Ag ₅ ...DBC	-1754792.073	-16.05
Ag ₆	-548561.5001	-1297658.429	Ag ₆ ...DBC	-1846238.533	-18.60
Ag ₇	-639994.219	-1297658.429	Ag ₇ ...DBC	-1937665.363	-12.71
Ag ₈	-731437.6883	-1297658.429	Ag ₈ ...DBC	-2029109.455	-13.33
Ag ₉	-822863.5367	-1297658.429	Ag ₉ ...DBC	-2120539.771	-17.80
Ag ₁₀	-914291.1658	-1297658.429	Ag ₁₀ ...DBC	-2211977.287	-27.69

Table S22. binding Energy (Kcal mol⁻¹) of most stable Ag_n...DBC (n=2-10) composites at M062X-D3.

Silver clusters	Ag _n (n=2-10), Energy (kcal mol ⁻¹)	DBC, Energy (kcal mol ⁻¹)	Ag _n ...DBC composite	Energy (kcal mol ⁻¹)	binding Energy (kcal mol ⁻¹)
Ag ₂	-182832.2305	-1297653.985	Ag ₂ ...DBC	-1480500.097	-13.88
Ag ₃	-274249.0072	-1297653.985	Ag ₃ ...DBC	-1571922.327	-19.33
Ag ₄	-365683.7278	-1297653.985	Ag ₄ ...DBC	-1663359.724	-22.01
Ag ₅	-457117.5363	-1297653.985	Ag ₅ ...DBC	-1754798.65	-27.12
Ag ₆	-548561.3531	-1297653.985	Ag ₆ ...DBC	-1846245.574	-30.23
Ag ₇	-639994.1678	-1297653.985	Ag ₇ ...DBC	-1937672.909	-24.75
Ag ₈	-731437.6053	-1297653.985	Ag ₈ ...DBC	-2029116.965	-25.37
Ag ₉	-822863.3396	-1297653.985	Ag ₉ ...DBC	-2120546.93	-29.60
Ag ₁₀	-914290.8409	-1297653.985	Ag ₁₀ ...DBC	-2211985.865	-41.03

Counterpoise corrected energies

Table S23. Counterpoise corrected energies of most stable Ag_n...DBC (n=2-10) composites calculated at M062X-D3/ LANL2DZ..

Silver clusters	Ag _n (n=2-10), Energy (Kcal mol ⁻¹)	DBC, Energy (Kcal mol ⁻¹)	Ag _n ...DBC composite	Counterpoise corrected Energy (Kcal mol ⁻¹)	binding Energy (Kcal mol ⁻¹)
Ag ₂	-182832.2305	-1297653.985	Ag ₂ ...DBC	-1480498.532	-12.31
Ag ₃	-274249.0072	-1297653.985	Ag ₃ ...DBC	-1571919.635	-16.64
Ag ₄	-365683.7278	-1297653.985	Ag ₄ ...DBC	-1663356.602	-18.88
Ag ₅	-457117.5363	-1297653.985	Ag ₅ ...DBC	-1754794.887	-23.36
Ag ₆	-548561.3531	-1297653.985	Ag ₆ ...DBC	-1846241.368	-26.02
Ag ₇	-639994.1678	-1297653.985	Ag ₇ ...DBC	-1937669.419	-21.26
Ag ₈	-731437.6053	-1297653.985	Ag ₈ ...DBC	-2029113.415	-21.82
Ag ₉	-822863.3396	-1297653.985	Ag ₉ ...DBC	-2120542.431	-25.10
Ag ₁₀	-914290.8409	-1297653.985	Ag ₁₀ ...DBC	-2211981.105	-36.27

GEOMETRIES OF Ag_n...DBC composites.

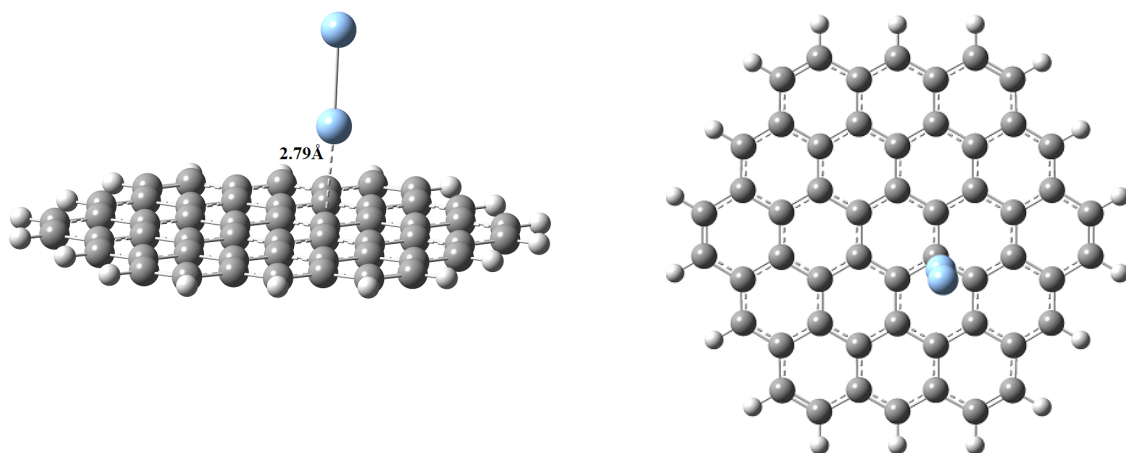


Figure S1. Top view (R) and side view (L) of Ag₂...DBC composites.

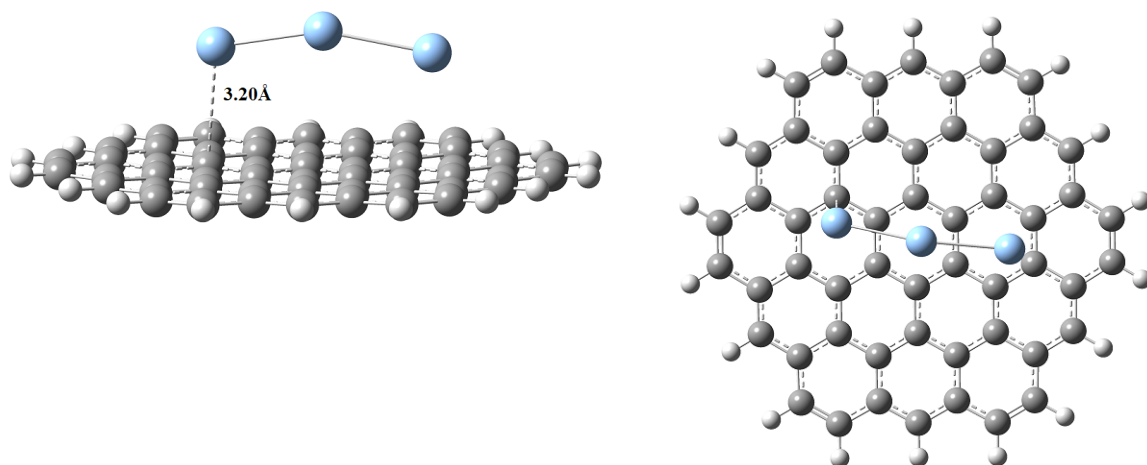


Figure S2. Top view (R) and side view (L) of Ag₃...DBC composites.

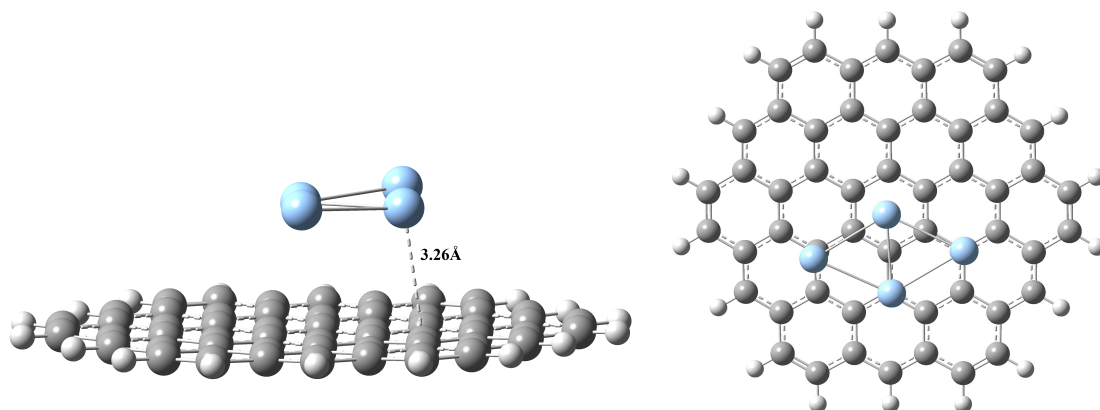


Figure S3. Top view (R) and side view (L) of Ag₄...DBC composites.

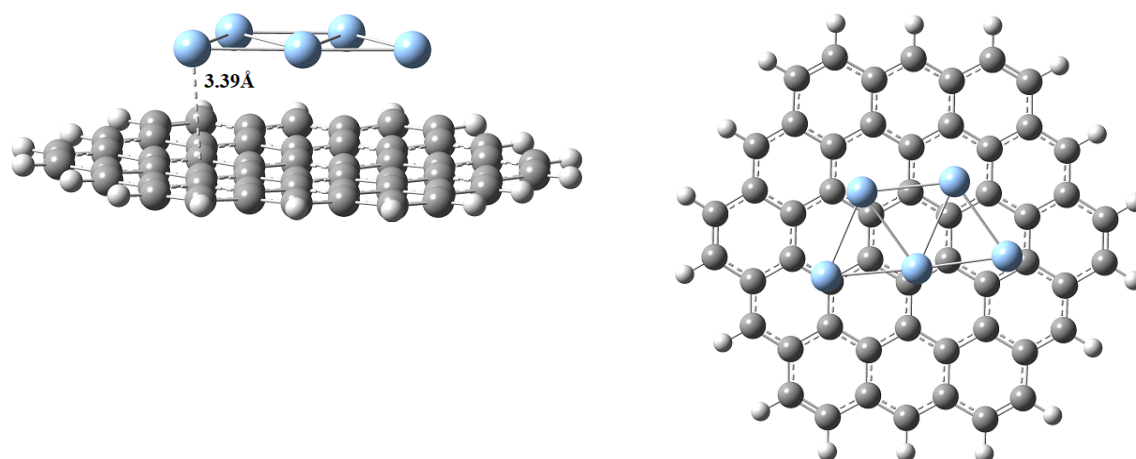


Figure S4. Top view (R) and side view (L) of Ag₅...DBC composites.

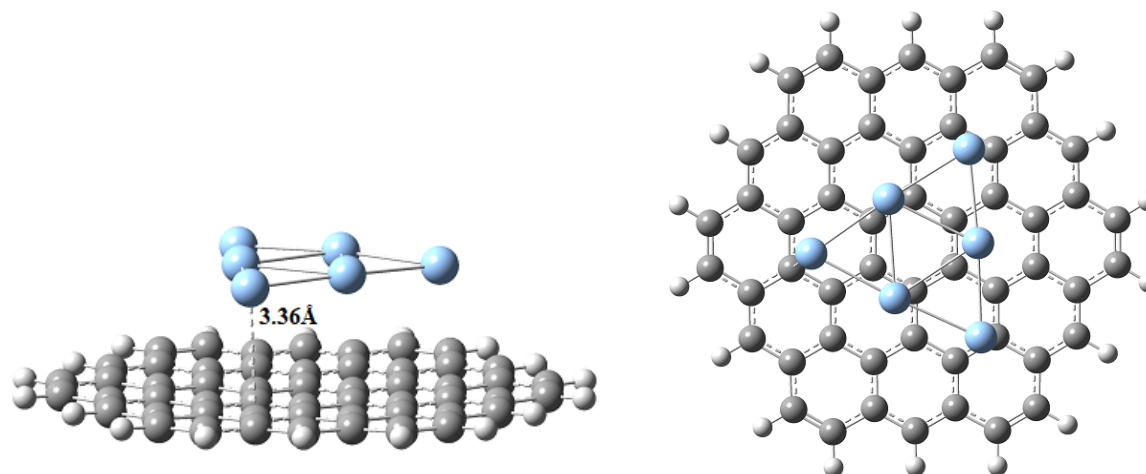


Figure S5. Top view (R) and side view (L) of Ag₆...DBC composites.

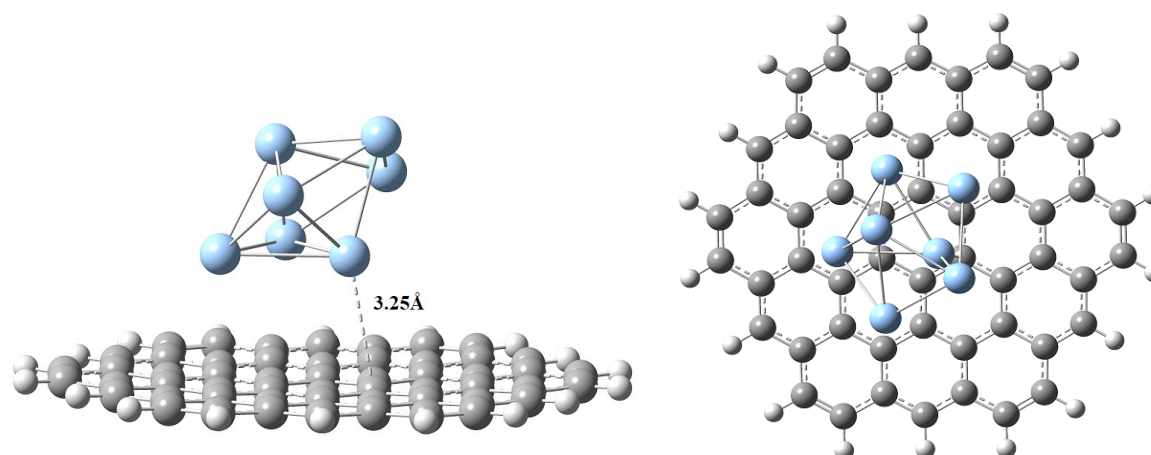


Figure S6. Top view (R) and side view (L) of Ag₇...DBC composites.

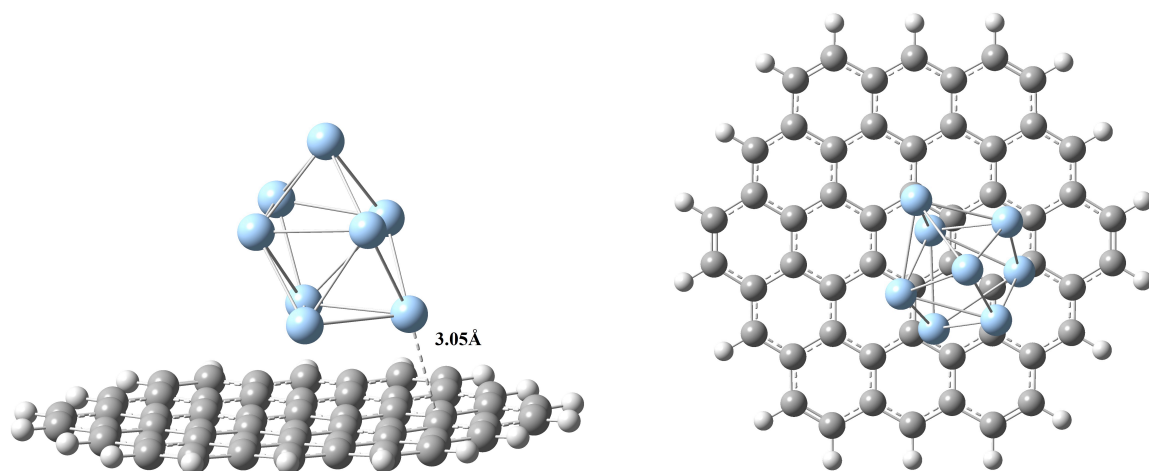


Figure S7. Top view (R) and side view (L) of Ag₈...DBC composites.

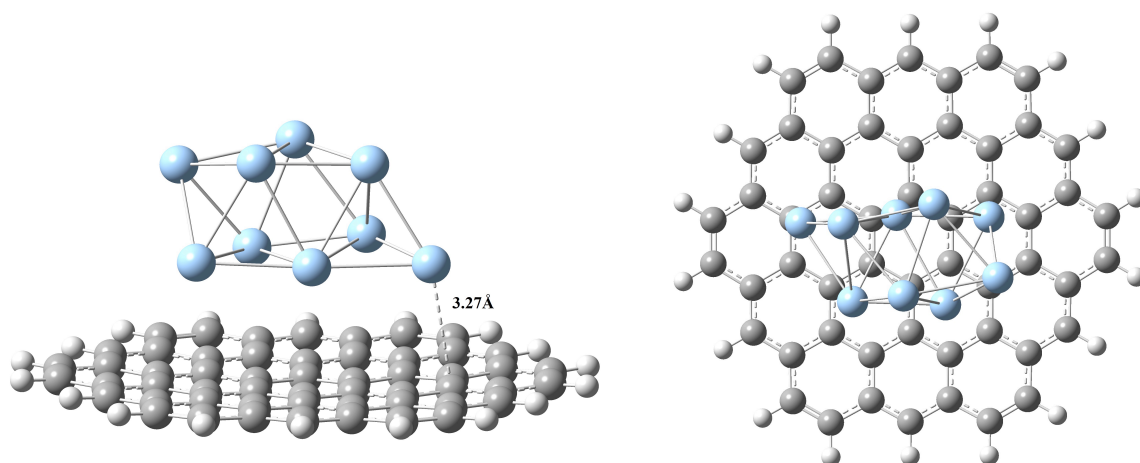


Figure S8. Top view (R) and side view (L) of Ag₉...DBC composites.

NON-COVALENT INTERACTIONS INDEX (NCI) ANALYSIS OF Ag_n...DBC.

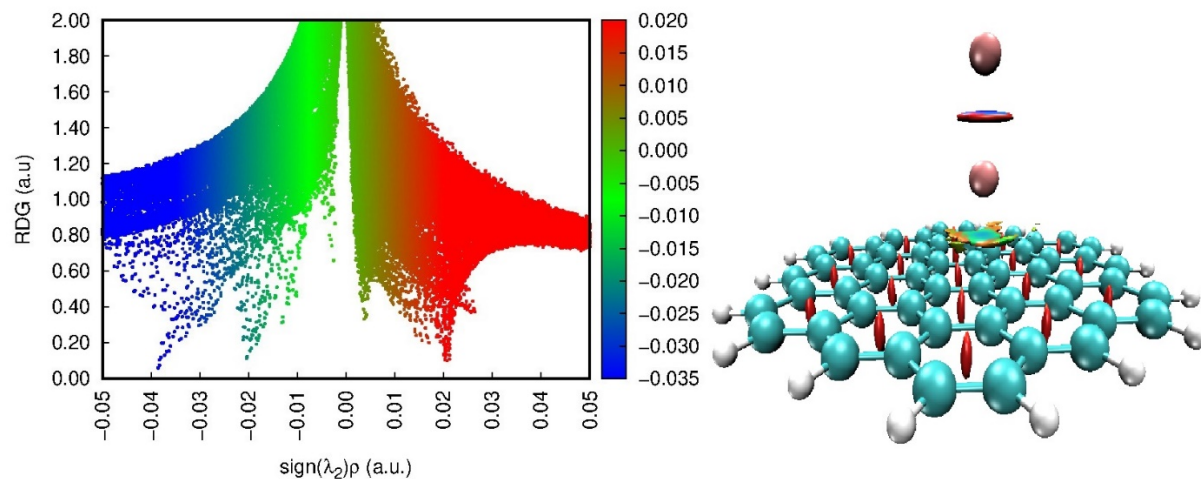


Figure S9. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for $\text{Ag}_2\text{...DBC}$.

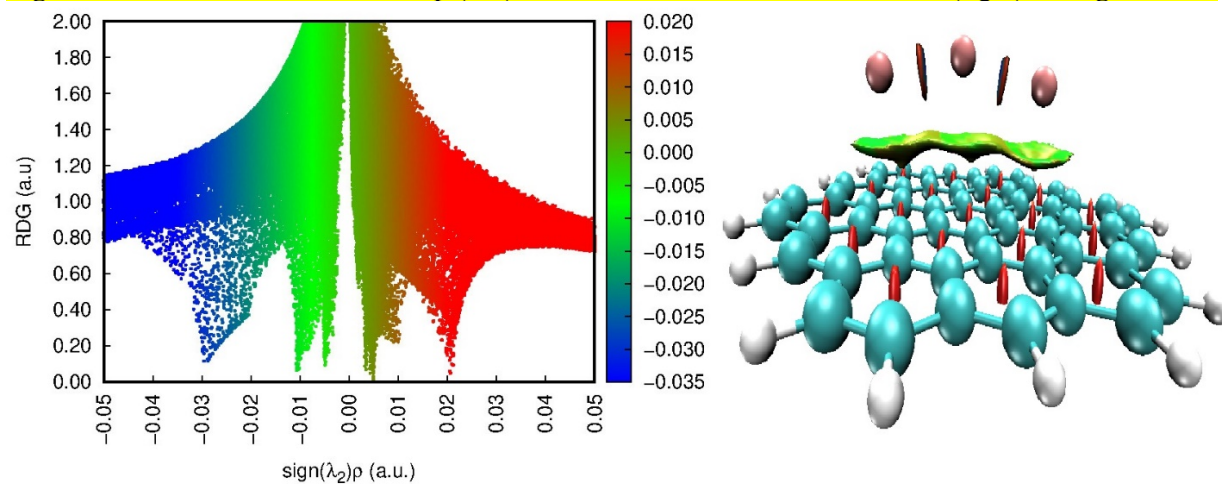


Figure S10. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for $\text{Ag}_3\text{...DBC}$.

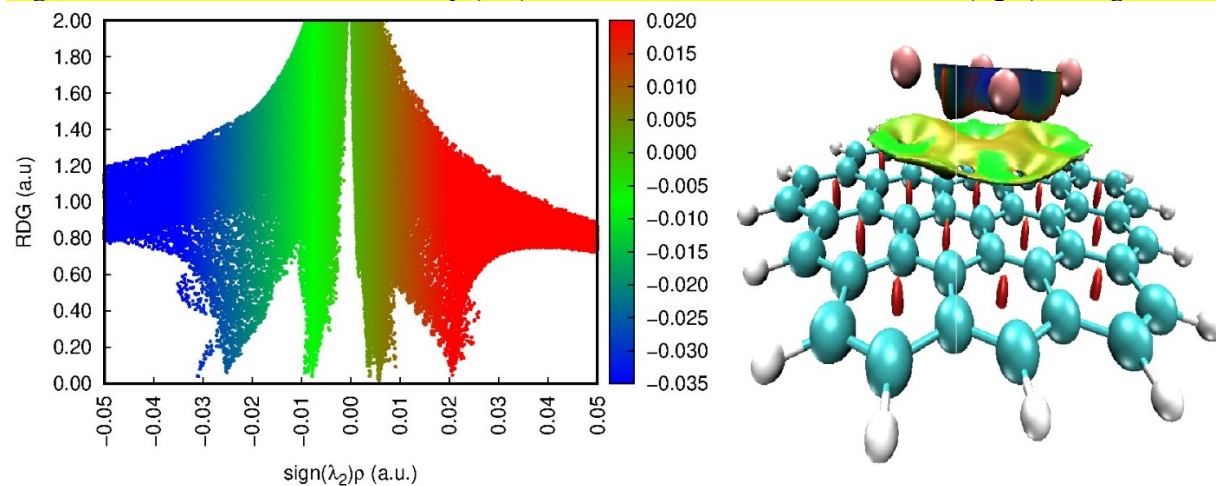


Figure S11. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for $\text{Ag}_4\text{...DBC}$.

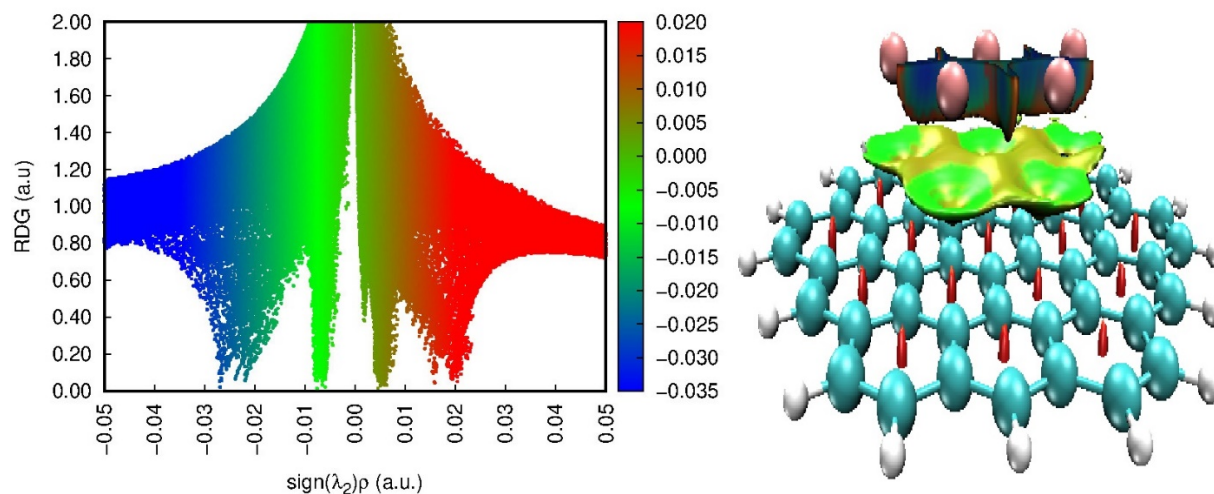


Figure S12. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for Ag₅...DBC.

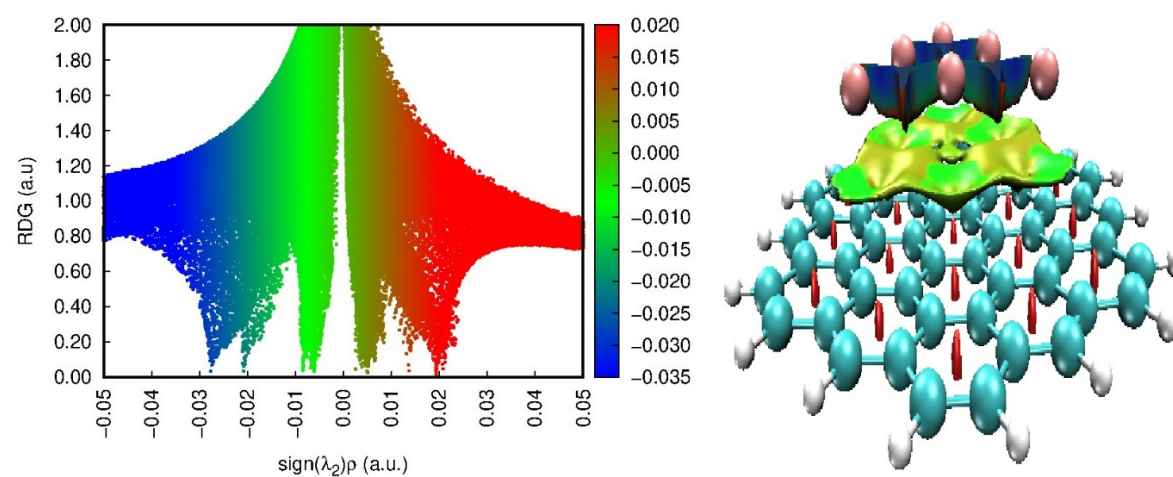


Figure S13. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for Ag₆...DBC.

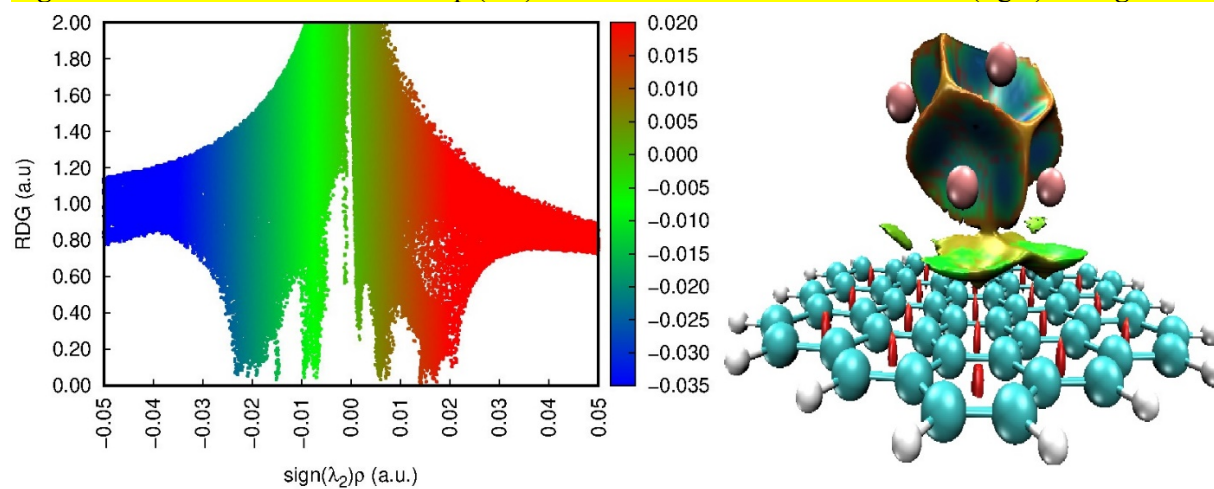


Figure S14. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for Ag₇...DBC.

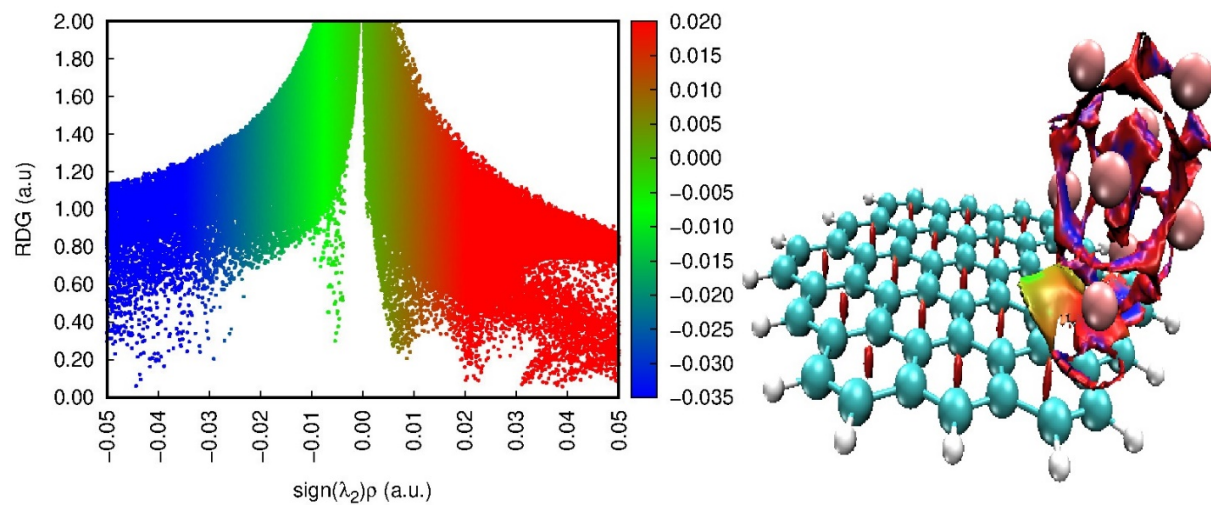


Figure S15. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for $\text{Ag}_8\text{...DBC}$.

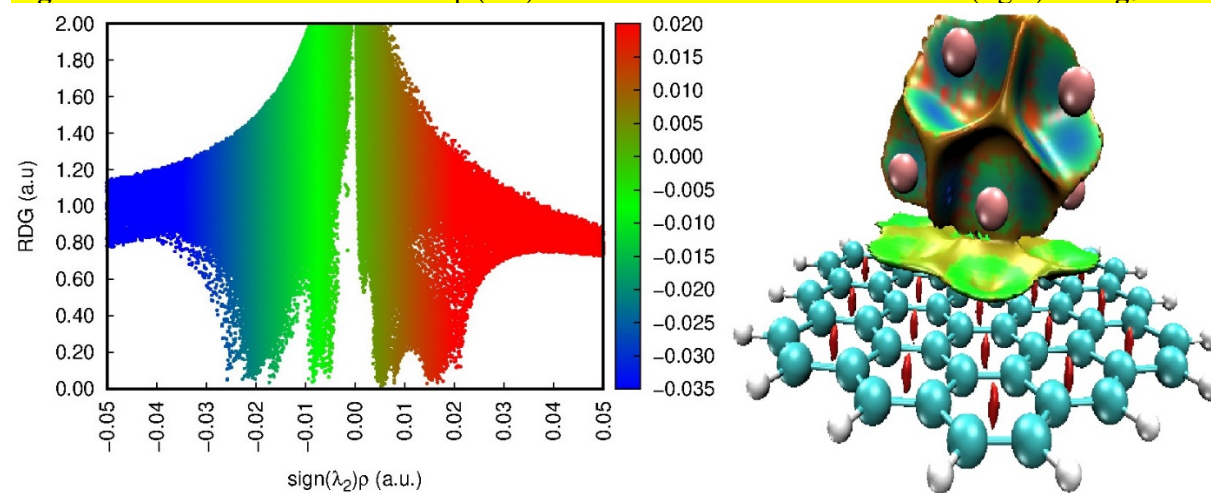
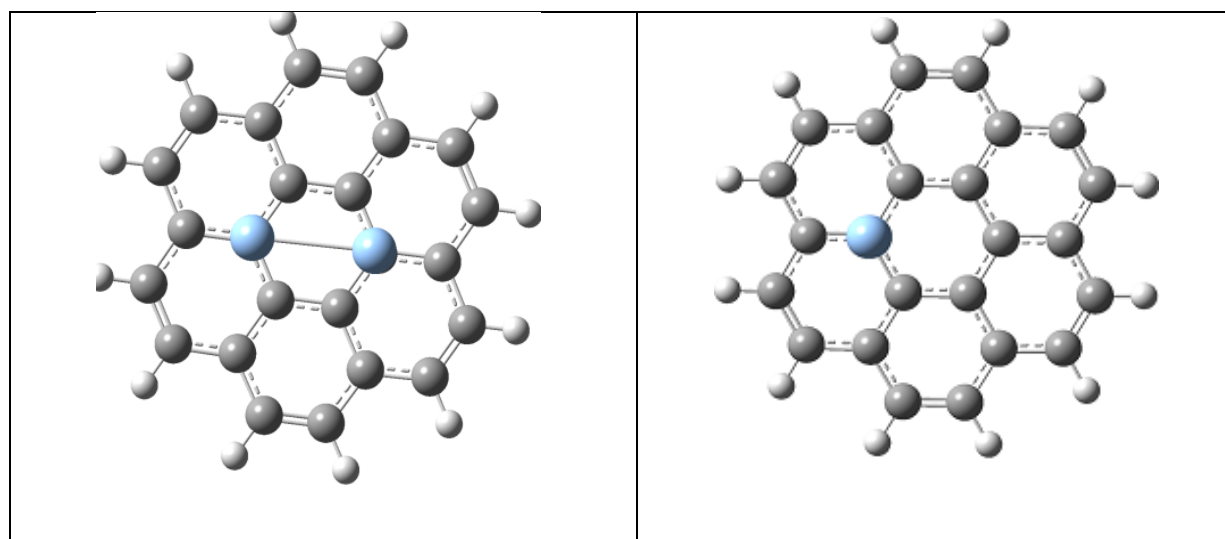
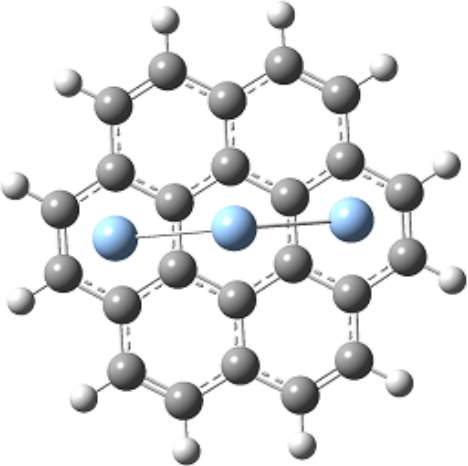
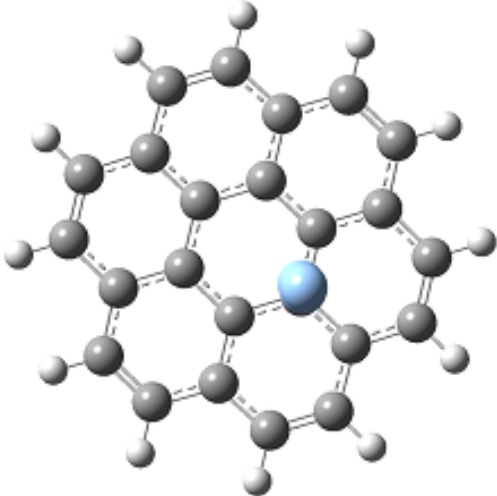
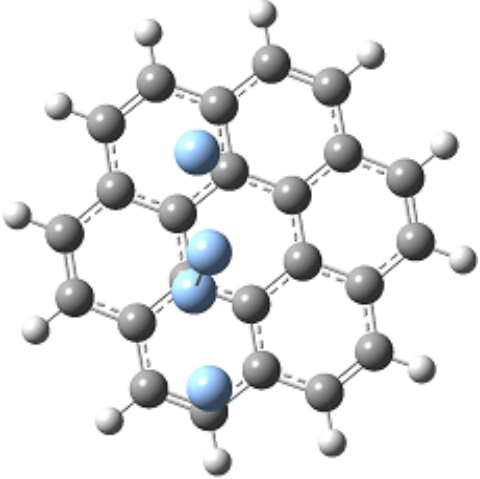
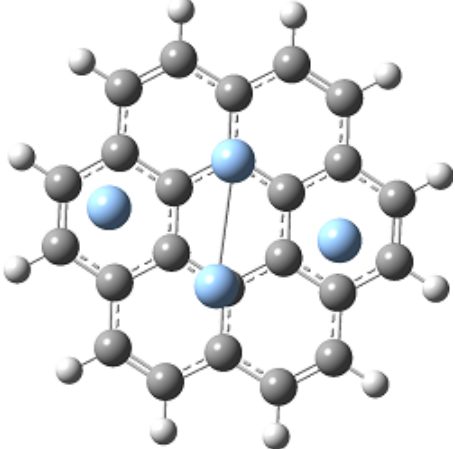
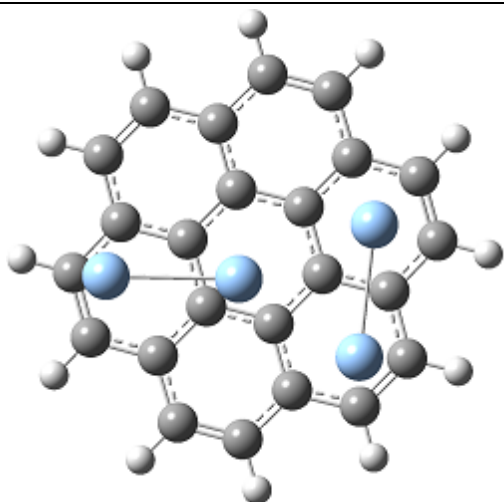


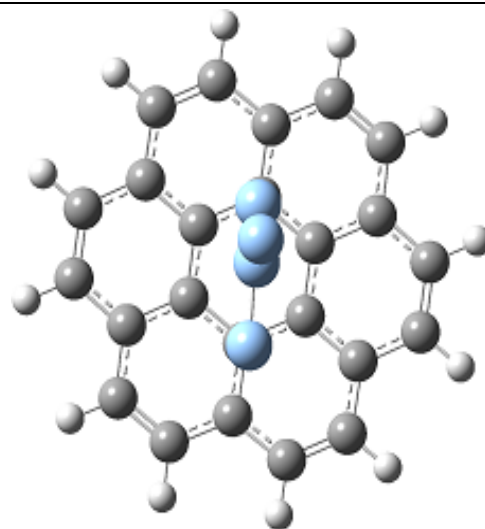
Figure S16. NCI-RDG 2D scatter map (left) and 3D color-filled RDG isosurface (right) for $\text{Ag}_9\text{...DBC}$.



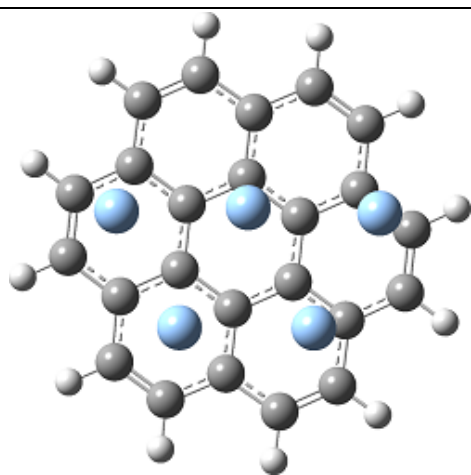
<p>$\text{Ag}_2 \parallel \dots\text{coronene (T)}$</p>	<p>$\text{Ag}_2 \perp \dots\text{coronene (T)}$</p>
 <p>A ball-and-stick model showing a coronene molecule (a polycyclic aromatic hydrocarbon with seven fused benzene rings) in a flat, horizontal orientation. Two silver atoms, represented by blue spheres, are positioned parallel to the plane of the coronene ring system, one on each side of the central cavity.</p>	 <p>A ball-and-stick model showing a coronene molecule in a flat, horizontal orientation. Two silver atoms, represented by blue spheres, are positioned perpendicular to the plane of the coronene ring system, one above and one below the central cavity.</p>
<p>$\text{a-Ag}_3 \dots\text{coronene (T)}$</p>	<p>$\text{b-Ag}_3 \dots\text{coronene (T)}$</p>
 <p>A ball-and-stick model showing a coronene molecule in a flat, horizontal orientation. Three silver atoms, represented by blue spheres, are positioned in a triangular arrangement within the central cavity of the coronene ring system.</p>	 <p>A ball-and-stick model showing a coronene molecule in a flat, horizontal orientation. Three silver atoms, represented by blue spheres, are positioned in a triangular arrangement within the central cavity of the coronene ring system, in a different orientation than the a-Ag3 model.</p>
<p>$\text{rh-Ag}_4 \perp \dots\text{coronene(T)}$</p>	<p>$\text{rh-Ag}_4 \parallel \dots\text{coronene(T)}$</p>



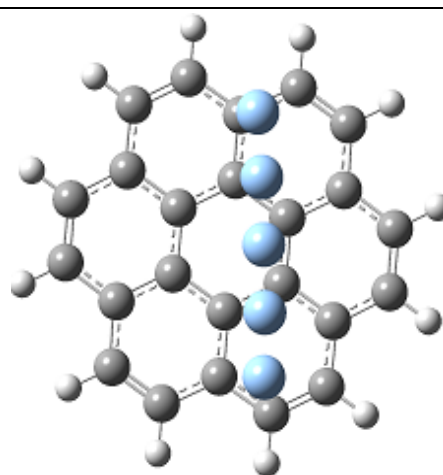
Υ -Ag₄ || ...coronene(T)



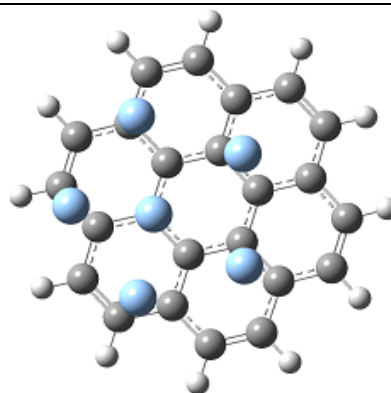
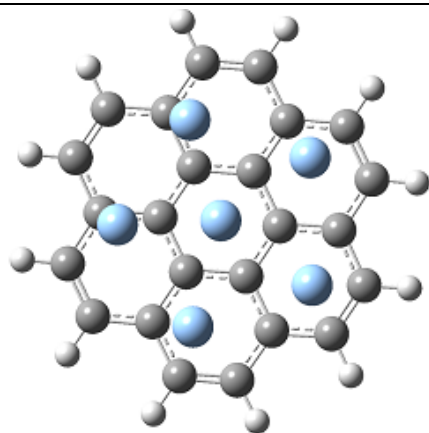
YAg₄⊥...coronene(T)

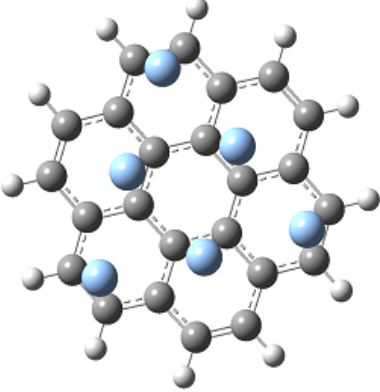
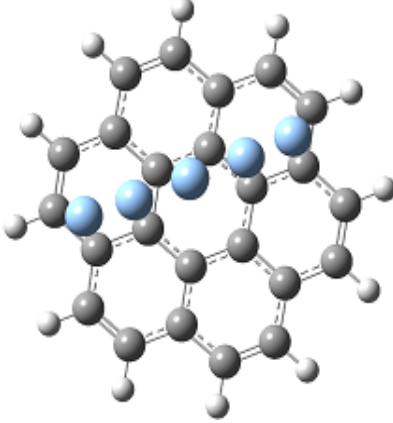
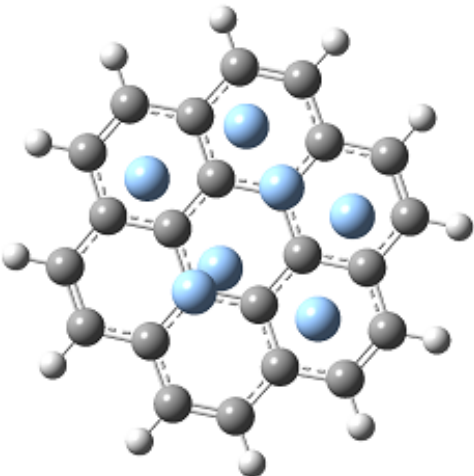
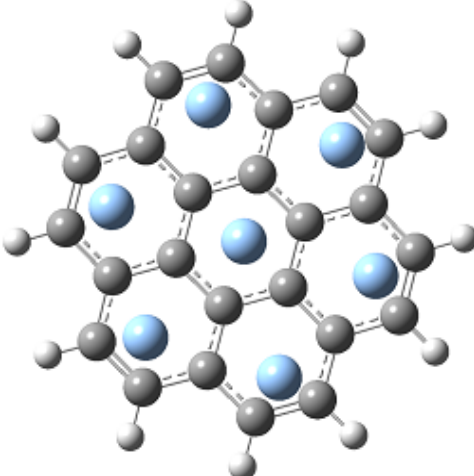


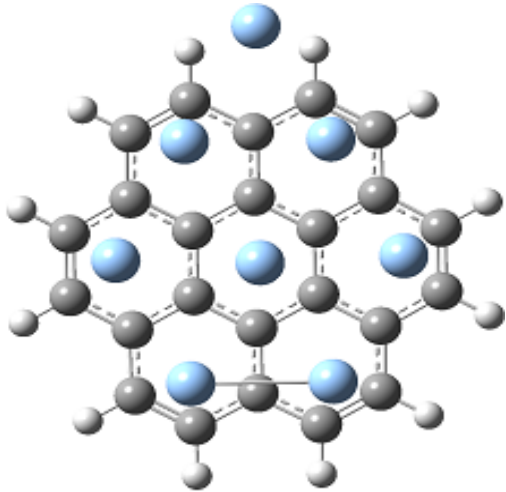
a-Ag₅...coronene(T)



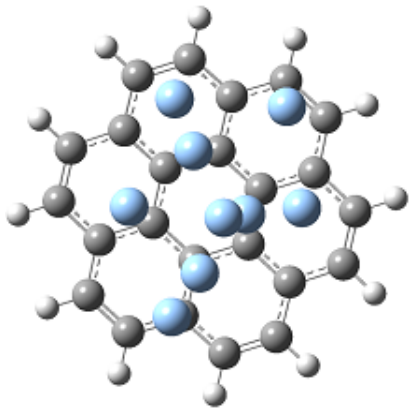
b-Ag₅...coronene(T)



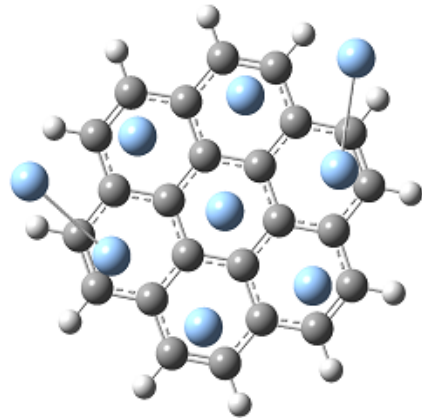
<p>a-Ag₆...coronene(T)</p>	<p>b-Ag₆...coronene(T)</p>
	
<p>c-Ag₆...coronene(T)</p>	<p>d-Ag₆...coronene(T)</p>
	
<p>a-Ag₇...coronene(T)</p>	<p>b-Ag₇...coronene(T)</p>



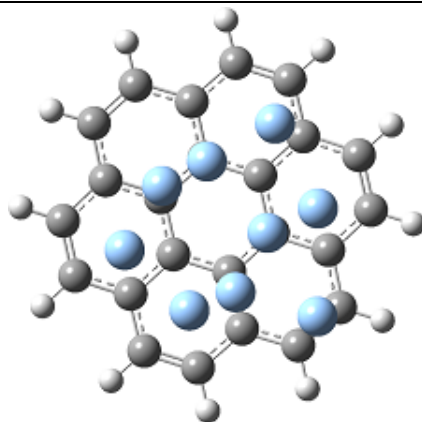
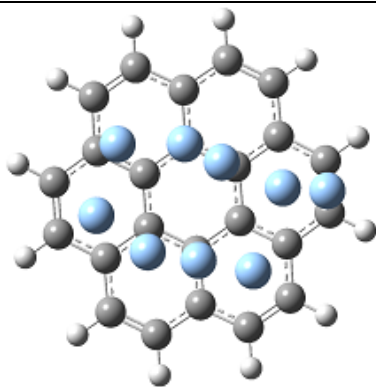
a-Ag₈...coronene(T)



a-Ag₉...coronene(T)



b-Ag₉...coronene(T)



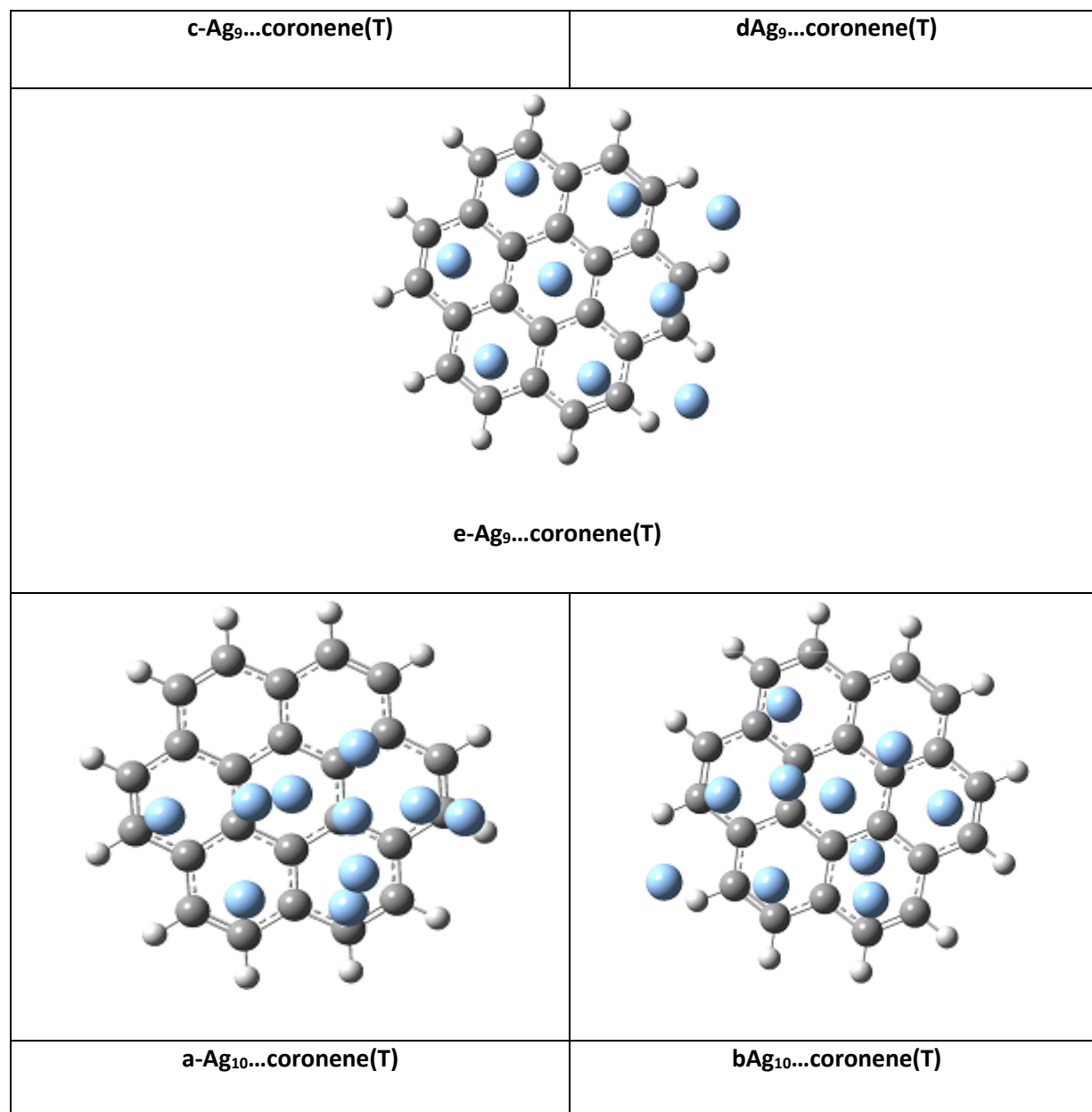


Figure S17. Top view of Ag_n---Coronene clusters optimized at M06-2X/LANL2DZ level of theory
COORDINATES FOR SILVER CLUSTERS (Ag_n, n=2-10) OVER COORONENE AT VARIOUS
POSSIBLE ORIENTATIONS

a-Ag₂...Coronene

C	1.37778067	3.22555768	-1.33194537
C	1.72901960	1.90717480	-0.89727965
C	0.69563643	0.98913185	-0.57986361
C	2.38098008	-0.72827983	-0.02804867

C	1.02349277	-0.33518849	-0.14321110
C	2.68509373	-2.05703089	0.41033600
C	0.30413005	-2.57356932	0.60941850
C	-0.75565051	-3.48373579	0.92404943
C	-0.02043263	-1.26260223	0.17735196
C	-2.07397483	-3.10225525	0.81228092
H	-0.49920941	-4.48634514	1.25428829
C	-1.39181990	-0.86557972	0.06094753
C	-2.42520945	-1.78374233	0.37801245
H	-2.87072852	-3.80024335	1.05327381
C	-1.71968078	0.45874847	-0.37568961
C	-3.78893456	-1.36487028	0.25426550
C	-3.07716816	0.85178498	-0.49100982
C	-0.67575574	1.38615400	-0.69627418
C	-4.10390305	-0.09184386	-0.16548557
H	-4.57466491	-2.07392475	0.49897298
C	-3.38128271	2.18047848	-0.92957031
C	-1.00032023	2.69700850	-1.12868161
H	-5.14147299	0.21674671	-0.25628991
C	-2.37792999	3.07184999	-1.23760866
H	-4.42353373	2.47432045	-1.01542391
H	-2.61856975	4.07778816	-1.56958588
C	1.68173555	-2.94844263	0.71825501
C	0.05945555	3.60704117	-1.44370853
C	3.40771106	0.21529339	-0.35374091
C	3.09274391	1.48827717	-0.77361272
H	1.92237220	-3.95446822	1.04997256
H	-0.19699079	4.60949620	-1.77441453
H	2.17453074	3.92338555	-1.57341610
H	3.87847340	2.19725126	-1.01855799

H	4.44528092	-0.09332601	-0.26301973
H	3.72734606	-2.35089450	0.49608718
Ag	0.89417599	0.02416422	-3.62085076
Ag	-1.03123647	-1.73877805	-3.00311829

b-Ag₂...coronene

C	-3.26665600	2.75534400	-1.45995000
C	-2.35256300	2.61703700	-0.36684600
C	-1.98597800	1.31638800	0.06212000
C	-0.53103500	2.29624200	1.80258100
C	-1.07531900	1.15688700	1.15653200
C	0.38637900	2.10784500	2.88648900
C	0.21135400	-0.32245000	2.66764500
C	0.57350200	-1.64691700	3.07704100
C	-0.69367500	-0.16133700	1.58200600
C	0.05294600	-2.75207600	2.44118800
H	1.27483300	-1.76302800	3.89790800
C	-1.24514400	-1.31453000	0.92928100
C	-0.86786300	-2.61470000	1.35265300
H	0.33928000	-3.75118900	2.75629500
C	-2.15497300	-1.14980200	-0.16431400
C	-1.41814100	-3.75047100	0.67701100
C	-2.68954800	-2.28939100	-0.81600500
C	-2.53084500	0.16446600	-0.59212600
C	-2.29846800	-3.59275500	-0.36993800
H	-1.12474100	-4.74335500	1.00495000
C	-3.60074500	-2.10256700	-1.90433900
C	-3.43119900	0.32550400	-1.67510600
H	-2.70933700	-4.46063700	-0.87772400
C	-3.95859400	-0.83927300	-2.31936900
H	-4.00525000	-2.97984900	-2.40081600

H	-4.64939800	-0.70772200	-3.14714800
C	0.74390700	0.84524000	3.30571500
C	-3.78751400	1.64831200	-2.09166100
C	-0.91341800	3.59906600	1.34941400
C	-1.79349700	3.75322200	0.30174400
H	1.44446000	0.71482900	4.12507500
H	-4.47900900	1.76350700	-2.92131200
H	-3.54154100	3.75450300	-1.78523100
H	-2.07537600	4.74594500	-0.03703700
H	-0.49122300	4.46747300	1.84652100
H	0.80259000	2.98504600	3.37300600
Ag	3.76384600	0.04791900	-1.59750200
Ag	1.57609500	-0.05475400	-0.03707400

a-Ag₃...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800

C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	0.25955533	1.08382970	2.57951233
Ag	2.67801424	2.11981427	2.26617029
Ag	-2.15890358	0.04784513	2.89285437

b-Ag₃...Coronene

C	3.08660100	3.74529200	-0.31405400
C	2.74753300	2.80548500	0.71083700
C	2.75323200	1.42255100	0.40090100
C	2.06761700	0.90209600	2.71640900
C	2.41815100	0.46387900	1.41236700
C	1.70246700	-0.07343500	3.69996900

C	2.01017800	-1.88474200	2.08381200
C	1.96816600	-3.27162700	1.73049900
C	2.37570000	-0.93494900	1.09129700
C	2.29371500	-3.69128000	0.46155800
H	1.67169200	-3.98612000	2.49193300
C	2.71149900	-1.37418800	-0.23452600
C	2.67374000	-2.75521700	-0.55395300
H	2.26066100	-4.74589800	0.20665000
C	3.06993400	-0.41452300	-1.23750000
C	3.02328000	-3.17087800	-1.87813700
C	3.40232300	-0.84952100	-2.54502900
C	3.08754600	0.98179500	-0.91956500
C	3.38114500	-2.25053500	-2.83792800
H	3.00446400	-4.23085000	-2.11172200
C	3.75001100	0.12600500	-3.53363900
C	3.41818300	1.93214000	-1.91910800
H	3.64320500	-2.57153800	-3.84127200
C	3.76041700	1.46913100	-3.22990100
H	4.00819600	-0.21493600	-4.53177600
H	4.02147200	2.19814900	-3.99053000
C	1.67751900	-1.41756700	3.39675000
C	3.41096200	3.32368700	-1.58363100
C	2.05461800	2.30495200	3.00076400
C	2.39068900	3.22503700	2.03285400
H	1.37838000	-2.14080200	4.14864600
H	3.66805900	4.04079100	-2.35671700
H	3.08013700	4.80394800	-0.07471600
H	2.37139400	4.28640400	2.25939600
H	1.77091300	2.63560400	3.99462800
H	1.41938000	0.26846200	4.69085100

Ag	-3.02086400	-0.09024100	-0.08652400
Ag	-5.66887800	0.32424400	-0.66446400
Ag	-0.32534900	-0.31963600	0.48308100

a-Ag₄...Coronene

C	-2.69374900	1.96547900	2.61547500
C	-1.95916600	0.73763700	2.64115700
C	-2.01830600	-0.12106400	1.51419000
C	-0.44672400	-1.68545000	2.62058000
C	-1.24567700	-1.33207200	1.49622700
C	0.29878900	-2.90939600	2.58456300
C	-0.54397600	-3.40347700	0.34076100
C	-0.59358000	-4.24022200	-0.81978100
C	-1.29664200	-2.20026800	0.35094000
C	-1.35588500	-3.89070500	-1.91186200
H	-0.01051000	-5.15627500	-0.82582200
C	-2.08815000	-1.83436100	-0.78642300
C	-2.12239800	-2.68112800	-1.92291000
H	-1.38180600	-4.52951500	-2.78996700
C	-2.84378100	-0.61799600	-0.77317800
C	-2.91433200	-2.29504100	-3.05161100
C	-3.61049200	-0.24981400	-1.90734400
C	-2.80410400	0.24056700	0.37258100
C	-3.63108200	-1.11933300	-3.04454700
H	-2.93439000	-2.94576600	-3.92093200
C	-4.33620700	0.98409800	-1.88502700
C	-3.52619000	1.46014900	0.37080300
H	-4.22270000	-0.83106000	-3.90871200
C	-4.29398800	1.81177200	-0.78552500
H	-4.91839000	1.26149200	-2.75903100
H	-4.84010100	2.75060200	-0.78156200

C	0.24834100	-3.73860700	1.48612300
C	-3.44814700	2.31595700	1.51723700
C	-0.41333200	-0.80307500	3.74993300
C	-1.14306300	0.36494300	3.75814900
H	0.82607700	-4.65773700	1.46691900
H	-3.99485000	3.25441600	1.50353500
H	-2.63683200	2.62481600	3.47650600
H	-1.10227100	1.02964900	4.61596700
H	0.20536100	-1.07292200	4.60060300
H	0.91310700	-3.16844400	3.44159400
Ag	-0.24203900	2.54241500	-0.30910100
Ag	0.94606300	-0.16717200	0.42012000
Ag	3.61839200	-0.90599800	-0.33669500
Ag	2.41776300	1.74116300	-0.95096600

b-Ag₄...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100

C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-0.40572854	2.74838420	-1.97820915
Ag	0.97984369	0.33219597	-1.58310856
Ag	-0.30170252	-2.14448430	-1.21219801
Ag	-1.68727083	0.27165576	-1.60760683

c-Ag₄...Coronene

C	0.52275008	3.07407517	0.55749589
C	1.20745908	1.83931817	0.79456389
C	0.45441308	0.69131017	1.14935989
C	2.52666108	-0.64865683	1.23895489

C	1.11679808	-0.55915583	1.37366889
C	3.16546308	-1.91345083	1.44820589
C	1.00813608	-2.96588583	1.91459689
C	0.22403408	-4.12168783	2.23026789
C	0.35472708	-1.72279683	1.71848989
C	-1.14674592	-4.04175283	2.32814789
H	0.73198008	-5.06992783	2.38086689
C	-1.07077692	-1.63899683	1.82364489
C	-1.82861692	-2.80040483	2.11961089
H	-1.73422092	-4.92625983	2.55720289
C	-1.73409792	-0.39145783	1.58581789
C	-3.25605592	-2.70211283	2.18123489
C	-3.15036592	-0.31792683	1.64775789
C	-0.97106892	0.77481517	1.25315289
C	-3.89497092	-1.50336783	1.95275089
H	-3.82950392	-3.59669283	2.40685889
C	-3.79359292	0.93561017	1.38985089
C	-1.62968492	2.00434817	0.99897689
H	-4.97867692	-1.44025683	1.99656089
C	-3.05853492	2.05784517	1.07902889
H	-4.87776492	0.98360417	1.44024089
H	-3.55573892	3.00336117	0.88229489
C	2.43190208	-3.03269083	1.77387489
C	-0.84818392	3.15382917	0.65561989
C	3.26727508	0.52530517	0.88579189
C	2.62984408	1.72714317	0.67229889
H	2.92504108	-3.98873483	1.92478689
H	-1.35994992	4.09286017	0.46539589
H	1.10677308	3.94981417	0.28909789
H	3.19979308	2.61127117	0.40105889

H	4.34642308	0.44941117	0.78559889
H	4.24490208	-1.97466183	1.34130289
Ag	0.98299985	0.49728327	-1.75685597
Ag	0.71315401	-2.18397493	-0.94944151
Ag	-1.77167721	-3.46995899	-0.65662886
Ag	-1.50181939	-0.78879180	-1.46434150

d-Ag₄...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400

C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	0.30120148	0.44527118	-2.36311064
Ag	-1.13592207	2.56300751	-2.83545616
Ag	2.75490236	-0.86110533	-2.04285380
Ag	0.58017408	-2.27921635	-1.78436310

f-Ag₄...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800

C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-0.27931902	-0.46292551	-2.08881233
Ag	-1.48333814	1.78294789	-2.61761494
Ag	2.02146543	-2.00646881	-1.69677022
Ag	-0.29110123	-3.19386541	-1.47445481

g-Ag₄...Coronene

C	0.80673797	4.27506106	1.09725937
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C	1.60311856	3.10459872	1.31044557
C	0.96216411	1.89115156	1.66766292
C	3.14696837	0.74103404	1.70779508
C	1.73747839	0.70314900	1.86834004
C	3.89979685	-0.46322777	1.89369999
C	1.85394160	-1.70783236	2.38830642
C	1.18203105	-2.93151002	2.70688384
C	1.08874610	-0.52659627	2.21559654
C	-0.18836718	-2.97514160	2.82981836
H	1.77522791	-3.83172538	2.83946621
C	-0.33635864	-0.57132498	2.34681198
C	-0.98198120	-1.79808503	2.64516944
H	-0.69026891	-3.91037006	3.06087696
C	-1.11259425	0.61378478	2.13260850
C	-2.41111139	-1.82821160	2.73303418
C	-2.52838558	0.55999263	2.22035664
C	-0.46291763	1.84614169	1.79751346
C	-3.15851750	-0.68959183	2.52727700
H	-2.89820954	-2.77219227	2.96031828
C	-3.28551746	1.75302908	1.98577751
C	-1.23316451	3.01386664	1.56671038
H	-4.24253577	-0.72390597	2.59090051
C	-2.65936335	2.93885500	1.67260044
H	-4.36852966	1.70356562	2.05584487
H	-3.24247407	3.83767898	1.49367604
C	3.27514127	-1.64605346	2.22172285
C	-0.56379296	4.23123354	1.22043887
C	3.77325789	1.97920700	1.35267660
C	3.02733128	3.12092232	1.16191034
H	3.85429453	-2.55536680	2.35480698

H	-1.16070620	5.12224651	1.04822011
H	1.30525567	5.20155702	0.82684398
H	3.51103266	4.05453827	0.88898260
H	4.85283334	2.00082465	1.23264136
H	4.97822827	-0.42690767	1.76708992
Ag	-0.27611339	-0.54154087	-3.50110374
Ag	-0.54230290	-1.11701469	-6.02523024
Ag	0.60406800	1.10400742	-1.41608970
Ag	-0.65087836	-1.09398471	-0.78265496

h-Ag₄...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200

C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	0.08321270	0.94193532	-1.50865757
Ag	1.36782770	-0.34267968	-4.28818957
Ag	-1.20140230	-0.34267968	-4.28818957
Ag	0.08321270	-1.62729468	-1.50865757

i-Ag₄...Coronene

C	1.35835618	3.74481165	-0.26410578
C	1.94240026	2.46184899	-0.01400216
C	1.09816175	1.37666282	0.33314787
C	3.05941825	-0.11872349	0.45579922
C	1.65891692	0.07971077	0.57021887
C	3.59576801	-1.42819969	0.67751722
C	1.35738420	-2.30941553	1.11603330
C	0.48213035	-3.40012629	1.42364203
C	0.80461456	-1.02040375	0.90730882

C	-0.87963183	-3.21438188	1.50181283
H	0.91326435	-4.38412669	1.58400096
C	-0.61150665	-0.82655951	0.99196562
C	-1.46073661	-1.92495872	1.28025980
H	-1.53672699	-4.05009328	1.72487807
C	-1.17323197	0.46749528	0.74137262
C	-2.87706115	-1.71668125	1.32132359
C	-2.58033433	0.65022561	0.78297791
C	-0.31794127	1.57020609	0.41644393
C	-3.41834994	-0.47312107	1.08055103
H	-3.52090159	-2.56352996	1.54118472
C	-3.12128443	1.94863543	0.51257645
C	-0.87613674	2.84588401	0.14961905
H	-4.49446436	-0.32648645	1.10878315
C	-2.29758068	3.00967863	0.20920961
H	-4.19912140	2.08025897	0.54742200
H	-2.71757166	3.98996046	0.00288053
C	2.77358037	-2.48631605	0.99574270
C	-0.00357690	3.93038840	-0.18569270
C	3.89324227	0.99330386	0.11003535
C	3.35346218	2.23989012	-0.11573502
H	3.18934657	-3.47695447	1.15622518
H	-0.43867622	4.90535184	-0.38570197
H	2.01188297	4.57189848	-0.52653533
H	3.99364508	3.07641517	-0.38122893
H	4.96461394	0.83406242	0.02539580
H	4.66865610	-1.57284974	0.58613293
Ag	0.99723674	1.30407539	-2.54906494
Ag	-0.36208614	-1.17252301	-4.29404953
Ag	-1.35045535	-0.96170303	-1.93192675

Ag 1.96996874 -0.99376535 -1.93696759

a-Ag₅...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300

C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-0.11344593	0.39477250	-1.79941912
Ag	-0.33919533	-2.30579432	-1.18330519
Ag	2.16815147	-1.16429535	-1.50309744
Ag	-2.55564689	-0.74306403	-1.48205841
Ag	2.35036977	1.48868055	-2.10738029

b-Ag₅...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800

C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	0.24636528	0.62912022	-1.86900100
Ag	-2.19235229	-0.56284548	-1.27276722
Ag	0.14020774	-2.06009874	-1.17544657
Ag	-2.04789276	2.07419495	-1.95773890
Ag	2.51460177	-0.85632305	-1.76690198

c-Ag5...Coronene

C	1.57076777	4.67275375	2.64852558
C	2.25547677	3.43799675	2.88559358
C	1.50243077	2.28998875	3.24038958
C	3.57467877	0.95002175	3.32998458

C	2.16481577	1.03952275	3.46469858
C	4.21348077	-0.31477225	3.53923558
C	2.05615377	-1.36720725	4.00562658
C	1.27205177	-2.52300925	4.32129758
C	1.40274477	-0.12411825	3.80951958
C	-0.09872823	-2.44307425	4.41917758
H	1.77999777	-3.47124925	4.47189658
C	-0.02275923	-0.04031825	3.91467458
C	-0.78059923	-1.20172625	4.21064058
H	-0.68620323	-3.32758125	4.64823258
C	-0.68608023	1.20722075	3.67684758
C	-2.20803823	-1.10343425	4.27226458
C	-2.10234823	1.28075175	3.73878758
C	0.07694877	2.37349375	3.34418258
C	-2.84695323	0.09531075	4.04378058
H	-2.78148623	-1.99801425	4.49788858
C	-2.74557523	2.53428875	3.48088058
C	-0.58166723	3.60302675	3.09000658
H	-3.93065923	0.15842175	4.08759058
C	-2.01051723	3.65652375	3.17005858
H	-3.82974723	2.58228275	3.53127058
H	-2.50772123	4.60203975	2.97332458
C	3.47991977	-1.43401225	3.86490458
C	0.19983377	4.75250775	2.74664958
C	4.31529277	2.12398375	2.97682158
C	3.67786177	3.32582175	2.76332858
H	3.97305877	-2.39005625	4.01581658
H	-0.31193223	5.69153875	2.55642558
H	2.15479077	5.54849275	2.38012758
H	4.24781077	4.20994975	2.49208858

H	5.39444077	2.04808975	2.87662858
H	5.29291977	-0.37598325	3.43233258
Ag	2.74941702	0.30474142	0.31988088
Ag	0.34346163	-0.79076814	1.17711934
Ag	0.46796242	1.88566639	0.46068884
Ag	2.60418692	-2.31070536	1.02562994
Ag	2.84615417	2.92557345	-0.37563628

d-Ags...Coronene

C	1.63724266	4.70147267	2.88281917
C	2.32195166	3.46671567	3.11988717
C	1.56890566	2.31870767	3.47468317
C	3.64115366	0.97874067	3.56427817
C	2.23129066	1.06824167	3.69899217
C	4.27995566	-0.28605333	3.77352917
C	2.12262866	-1.33848833	4.23992017
C	1.33852666	-2.49429033	4.55559117
C	1.46921966	-0.09539933	4.04381317
C	-0.03225334	-2.41435533	4.65347117
H	1.84647266	-3.44253033	4.70619017
C	0.04371566	-0.01159933	4.14896817
C	-0.71412434	-1.17300733	4.44493417
H	-0.61972834	-3.29886233	4.88252617
C	-0.61960534	1.23593967	3.91114117
C	-2.14156334	-1.07471533	4.50655817
C	-2.03587334	1.30947067	3.97308117
C	0.14342366	2.40221267	3.57847617
C	-2.78047834	0.12402967	4.27807417
H	-2.71501134	-1.96929533	4.73218217
C	-2.67910034	2.56300767	3.71517417
C	-0.51519234	3.63174567	3.32430017

H	-3.86418434	0.18714067	4.32188417
C	-1.94404234	3.68524267	3.40435217
H	-3.76327234	2.61100167	3.76556417
H	-2.44124634	4.63075867	3.20761817
C	3.54639466	-1.40529333	4.09919817
C	0.26630866	4.78122667	2.98094317
C	4.38176766	2.15270267	3.21111517
C	3.74433666	3.35454067	2.99762217
H	4.03953366	-2.36133733	4.25011017
H	-0.24545734	5.72025767	2.79071917
H	2.22126566	5.57721167	2.61442117
H	4.31428566	4.23866867	2.72638217
H	5.46091566	2.07680867	3.11092217
H	5.35939466	-0.34726433	3.66662617
Ag	0.23127254	0.61151823	1.26469078
Ag	-1.03121378	-0.89876845	-0.69714070
Ag	0.47586584	1.31690206	-1.41239598
Ag	-1.24792596	-1.55970187	1.94108595
Ag	1.70014060	2.77470787	0.54019101

f-Ags...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100

H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-0.22569769	0.09429428	-1.26049467
Ag	2.05096002	-1.35538578	-1.19776207
Ag	2.12503296	1.29930592	-1.81789075
Ag	-2.50235325	1.54398008	-1.32322884

Ag -2.57642651 -1.11072330 -0.70309743

g-Ag5...Coronene

C	2.21204000	-3.56531200	1.55459400
C	2.35923100	-2.20662400	1.98218800
C	2.56365100	-1.20342100	1.00234300
C	2.59625800	0.51490400	2.77567000
C	2.68916700	0.16666800	1.40422300
C	2.67794900	1.89638700	3.15146800
C	2.90755700	2.54555200	0.81092400
C	3.04619500	3.55214000	-0.20308500
C	2.83905800	1.19186000	0.41293500
C	3.11855600	3.21893600	-1.53659000
H	3.08578500	4.59372900	0.10349400
C	2.91677100	0.84036400	-0.97593100
C	3.05410500	1.85381000	-1.95744200
H	3.22273300	3.99342600	-2.29082000
C	2.80652200	-0.52904400	-1.37500300
C	3.10923900	1.48399100	-3.33900400
C	2.85131900	-0.87304900	-2.75018600
C	2.63295000	-1.55092700	-0.38738700
C	3.01146800	0.16563900	-3.72218600
H	3.22253900	2.26698600	-4.08315900
C	2.71828000	-2.24736000	-3.12790700
C	2.48619800	-2.90328500	-0.78662300
H	3.04525400	-0.10597500	-4.77335700
C	2.53968300	-3.22878800	-2.17943900
H	2.74909800	-2.50312000	-4.18310000
H	2.42574900	-4.26700900	-2.47665800
C	2.82742500	2.88124200	2.20005400
C	2.27578200	-3.90157300	0.21906700

C	2.40487100	-0.52160100	3.74697900
C	2.29002000	-1.83941400	3.36380300
H	2.87051800	3.92765400	2.48847200
H	2.16280200	-4.93601400	-0.09114500
H	2.06025200	-4.33715700	2.30385000
H	2.13299100	-2.61760500	4.10496800
H	2.34088300	-0.24660500	4.79567500
H	2.60869700	2.15525000	4.20389700
Ag	-2.39989000	0.15946200	-0.09198500
Ag	-0.14067900	1.90345100	0.06476000
Ag	-2.82201300	2.98340600	-0.08712100
Ag	-3.18044200	-2.55277900	-0.26617700
Ag	-0.42576400	-1.90567100	0.34216300

h-Ag₅...Coronene

C	0.21114104	4.37505063	3.18816304
C	0.89341578	3.12127975	3.29867223
C	0.13187838	1.92918056	3.39787484
C	2.21119276	0.59989278	3.48270598
C	0.79345862	0.66177111	3.49124775
C	2.85101950	-0.67944063	3.55677091
C	0.67940316	-1.80006639	3.64325856
C	-0.10914301	-2.99394447	3.69976049
C	0.02419379	-0.54426790	3.57736181
C	-1.48426840	-2.93566507	3.67443081
H	0.40003427	-3.95199635	3.75194657
C	-1.40616467	-0.48351664	3.55443561
C	-2.16657898	-1.67978092	3.59326520
H	-2.07400465	-3.84732445	3.70658708
C	-2.06732497	0.78308666	3.44722965
C	-3.59496764	-1.59799130	3.52956870

C	-3.48415384	0.84040957	3.38113531
C	-1.29832202	1.98985099	3.37356624
C	-4.23180302	-0.38094023	3.42644601
H	-4.17022296	-2.51901527	3.55817519
C	-4.12350627	2.11612405	3.25706653
C	-1.95288928	3.24121096	3.24798051
H	-5.31572520	-0.32975954	3.37339642
C	-3.38359349	3.27589019	3.19539361
H	-5.20823436	2.15135059	3.20812216
H	-3.87760652	4.23842543	3.09847282
C	2.11111644	-1.83853658	3.63364893
C	-1.16415754	4.43311286	3.16303047
C	2.95970584	1.81733096	3.38787763
C	2.32285155	3.03512673	3.30011541
H	2.60567652	-2.80440711	3.68349961
H	-1.67316303	5.38817573	3.07009424
H	0.80137987	5.28411461	3.11563750
H	2.89919603	3.95286096	3.22470830
H	4.04473967	1.76221749	3.38307810
H	3.93670583	-0.71900935	3.54765464
Ag	-0.95096069	-0.87918185	0.07118544
Ag	0.62312456	1.31717325	-0.13467844
Ag	1.75124806	-1.08196037	0.03880088
Ag	-2.12258175	1.55816812	-0.10411198
Ag	-2.47463861	-0.46151047	-2.13064474

i-Ag₅...Coronene

C	0.87348231	4.29475061	3.27693492
C	1.48921116	3.00679663	3.38512481
C	0.66633346	1.85595898	3.48169510
C	2.67325141	0.41958231	3.56447798

C	1.26068988	0.55550158	3.57271500
C	3.24526840	-0.89160654	3.63615933
C	1.01798434	-1.89730089	3.71973160
C	0.16805921	-3.04841731	3.77358954
C	0.42937166	-0.60882655	3.65616634
C	-1.20212628	-2.91825273	3.74796084
H	0.62641617	-4.03188871	3.82399974
C	-0.99584303	-0.47330979	3.63292937
C	-1.81779238	-1.62824507	3.66911871
H	-1.83874472	-3.79788570	3.77810190
C	-1.58981660	0.82634821	3.52807495
C	-3.23992311	-1.47174042	3.60515450
C	-3.00168190	0.95781993	3.46166711
C	-0.75872705	1.99138951	3.45707561
C	-3.81219810	-0.22284700	3.50429089
H	-3.86256872	-2.36147537	3.63173131
C	-3.57339409	2.26546980	3.33997487
C	-1.34690627	3.27551697	3.33381275
H	-4.89193880	-0.11494504	3.45101623
C	-2.77381760	3.38507471	3.28086251
H	-4.65477561	2.35747343	3.29077304
H	-3.21677836	4.37231957	3.18573132
C	2.44573047	-2.01057303	3.71047811
C	-0.49688757	4.42470698	3.25150284
C	3.48444596	1.59639663	3.47232904
C	2.91218477	2.84600406	3.38682736
H	2.88908230	-3.00108328	3.75853274
H	-0.95521268	5.40526582	3.16033661
H	1.51048338	5.17184603	3.20641960
H	3.53576510	3.73249022	3.31344373

H	4.56511472	1.48462460	3.46774711
H	4.32740345	-0.98788063	3.62729219
Ag	-1.69879458	-0.34248253	-0.75231045
Ag	0.11103457	1.67378260	-0.80969876
Ag	-2.30265299	2.11888025	0.20745428
Ag	0.75706188	-0.81829137	-1.79465155
Ag	-0.19252417	-2.16664325	0.56969069

j-Ag₅...Coronene

C	0.68779266	3.29785673	3.26077049
C	1.28663471	2.00190830	3.36828040
C	0.44878546	0.86188775	3.46441895
C	2.43675301	-0.60065637	3.54627441
C	1.02609127	-0.44627542	3.55475578
C	2.99157857	-1.91924880	3.61727054
C	0.75134011	-2.89576189	3.70065868
C	-0.11356311	-4.03568738	3.75408822
C	0.17962416	-1.59966874	3.63777016
C	-1.48193185	-3.88759908	3.72869575
H	0.33189631	-5.02509373	3.80398070
C	-1.24369877	-1.44551002	3.61477897
C	-2.08068071	-2.58961171	3.65053455
H	-2.12999833	-4.75884345	3.75850780
C	-1.82063390	-0.13814470	3.51060721
C	-3.50065037	-2.41448816	3.58682552
C	-3.23066676	0.01181493	3.44444155
C	-0.97438460	1.01595888	3.44004518
C	-4.05655233	-1.15816877	3.48661810
H	-4.13487780	-3.29601475	3.61306682
C	-3.78523993	1.32688812	3.32343285
C	-1.54573127	2.30772782	3.31745699

H	-5.13479571	-1.03612743	3.43353208
C	-2.97109388	2.43596585	3.26474064
H	-4.86533145	1.43305205	3.27441246
H	-3.40111451	3.42896489	3.17012695
C	2.17748127	-3.02769579	3.69116947
C	-0.68076315	3.44573916	3.23557457
C	3.26326044	0.56548938	3.45457083
C	2.70738350	1.82251533	3.36972567
H	2.60784449	-4.02394301	3.73870502
H	-1.12623380	4.43225188	3.14492470
H	1.33620362	4.16657767	3.19058296
H	3.34249736	2.70080311	3.29667592
H	4.34237412	0.43959325	3.44979834
H	4.07236061	-2.02966548	3.60821988
Ag	-1.15415447	-0.57174191	-1.10537510
Ag	0.33105072	1.48017905	-0.14210672
Ag	-2.31780966	1.68485085	-0.15785424
Ag	1.54608727	-0.80142734	-1.09912001
Ag	-0.14406069	-2.53906095	0.46097933

a-Ag₆...Coronene

C	-3.80922000	-0.94291300	1.96216500
C	-3.01399300	0.24715100	2.00410500
C	-1.60401500	0.13030200	2.10081400
C	-1.39121600	2.59021400	2.07352800
C	-0.78842400	1.30799400	2.13670800
C	-0.55675000	3.75339200	2.10413000
C	1.44536900	2.35524300	2.23460400
C	2.86919100	2.21294300	2.27393000
C	0.63718000	1.18999100	2.21521200
C	3.45627600	0.96694200	2.30977400

H	3.48265400	3.10939100	2.26918000
C	1.24761800	-0.10587900	2.25603300
C	2.65979800	-0.22284900	2.31106600
H	4.53780500	0.86851400	2.33245600
C	0.43217100	-1.28327800	2.21864400
C	3.24893600	-1.52750600	2.34045200
C	1.03734900	-2.56589100	2.23927300
C	-0.99390600	-1.16520000	2.14581900
C	2.46437000	-2.66041400	2.30594300
H	4.33137400	-1.60982400	2.38512200
C	0.20459500	-3.72851900	2.16832300
C	-1.79984300	-2.33084300	2.09152400
H	2.91994700	-3.64659700	2.32268700
C	-1.16648000	-3.61477700	2.09713100
H	0.67528200	-4.70749000	2.16681800
H	-1.78989400	-4.50243600	2.03925600
C	0.81485700	3.63981000	2.18336400
C	-3.22205500	-2.18956400	2.00452500
C	-2.81525900	2.68362600	1.95892500
C	-3.59951300	1.55142200	1.92587600
H	1.44046100	4.52788100	2.20111300
H	-3.83354000	-3.08684000	1.96823800
H	-4.88897100	-0.84515700	1.89158900
H	-4.67898000	1.63343200	1.83597700
H	-3.26808800	3.66886000	1.89413600
H	-1.02517200	4.73262800	2.05862100
Ag	-1.33550100	0.98510100	-1.30485400
Ag	-0.04364600	-1.74674200	-1.22538300
Ag	1.68270900	0.74252900	-1.14566000
Ag	2.80774100	-1.88523900	-1.02450700

Ag	-2.88705700	-1.41831100	-1.29494400
Ag	0.36202800	3.28243200	-1.13947000

b-Ag₆...Coronene

C	2.35080600	0.61266300	3.71375000
C	2.58330300	1.38333000	2.52951400
C	2.87283900	0.71011500	1.31543200
C	3.03623300	2.87777400	0.14421300
C	3.10147300	1.46129000	0.11672500
C	3.26139600	3.60809000	-1.06665200
C	3.58565900	1.52357300	-2.30357000
C	3.81884900	0.82161500	-3.52910800
C	3.37518900	0.78078500	-1.11389600
C	3.85720100	-0.55533200	-3.56102700
H	3.96015700	1.39642500	-4.43993400
C	3.41855400	-0.65122100	-1.14640500
C	3.66723800	-1.32534000	-2.36897700
H	4.02785900	-1.07967100	-4.49689700
C	3.18848400	-1.40218200	0.05182100
C	3.69569300	-2.75682000	-2.38053300
C	3.21201700	-2.81989100	0.01564700
C	2.92031300	-0.72143100	1.28373100
C	3.47577500	-3.47943400	-1.22741500
H	3.88924300	-3.26681600	-3.32015300
C	2.94728700	-3.55030400	1.21840700
C	2.67567000	-1.46540600	2.46604200
H	3.49334900	-4.56558500	-1.24628300
C	2.68831300	-2.89560600	2.40253400
H	2.94946800	-4.63587500	1.18014700
H	2.48430600	-3.45823600	3.30904400
C	3.52839900	2.95330800	-2.25006000

C	2.39556300	-0.76492600	3.68303900
C	2.72549000	3.53520700	1.37749200
C	2.50710400	2.81311000	2.53027800
H	3.69311800	3.51552300	-3.16501700
H	2.21395700	-1.34119900	4.58595900
H	2.13306000	1.13577600	4.64075500
H	2.26929100	3.32172900	3.46022800
H	2.66079900	4.61949000	1.38670300
H	3.21312500	4.69309600	-1.03793000
Ag	-2.65586000	1.45515900	-0.18388400
Ag	-2.52143100	-1.56474200	-0.16667000
Ag	0.02050700	0.06123000	0.11242000
Ag	0.03867700	-2.79921500	0.16779400
Ag	-5.00946700	-0.16131400	-0.36098700
Ag	-0.21967800	2.91329800	0.17042200

c-Ag₆...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600

C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-0.35477136	-0.05712661	-1.64010537
Ag	-0.35477136	2.30157839	-3.01946037
Ag	-0.35477136	-2.41583161	-3.01946037
Ag	-2.71347636	-0.05712661	-3.01946037
Ag	2.00393364	-0.05712661	-3.01946037
Ag	-0.35477136	-0.05712661	-4.39881537

d-Ag₆...Coronene

C	1.76951064	4.02556312	-0.06036909
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C	2.12791065	2.67175267	0.23695093
C	1.10990151	1.75356126	0.59952890
C	2.79231926	-0.04275598	0.80068923
C	1.44317923	0.38943142	0.88379878
C	3.09964916	-1.41564785	1.06952764
C	0.73999523	-1.89797369	1.49213251
C	-0.30899026	-2.81768453	1.81478374
C	0.41289022	-0.54211254	1.23656573
C	-1.62157570	-2.40558262	1.86273553
H	-0.05026603	-3.85420887	2.01106764
C	-0.95202140	-0.11277975	1.28977570
C	-1.97637761	-1.04500192	1.59381852
H	-2.41180929	-3.11291868	2.09758076
C	-1.28656011	1.24823358	0.99205676
C	-3.33850427	-0.60277259	1.60304402
C	-2.64386505	1.66376695	1.00272256
C	-0.25502438	2.18255188	0.65138784
C	-3.66145103	0.70538134	1.31695732
H	-4.11748630	-1.32339087	1.83524754
C	-2.95693282	3.02499648	0.68546128
C	-0.58893488	3.52435908	0.33803647
H	-4.69828493	1.02984602	1.32133280
C	-1.96377691	3.92417852	0.36695700
H	-3.99805744	3.33516009	0.69684432
H	-2.21152757	4.95374736	0.12503921
C	2.10827975	-2.31173330	1.40282598
C	0.45672552	4.43753580	-0.01217349
C	3.80452162	0.90366538	0.43853873
C	3.48336873	2.21501942	0.16738656
H	2.35074369	-3.35223876	1.59914268

H	0.19310859	5.46457451	-0.24789878
H	2.55530790	4.72376287	-0.33437441
H	4.25762594	2.92464581	-0.11019493
H	4.83532239	0.56580251	0.37806233
H	4.13446913	-1.73959307	1.00192069
Ag	0.45546603	-1.17554751	-2.95004556
Ag	-1.35962752	-0.78196859	-0.94588974
Ag	0.45396536	0.50138274	-5.10736152
Ag	-1.97887173	-1.56078942	-4.12974798
Ag	1.07320957	1.28020357	-1.92350328
Ag	-1.36112819	0.89496166	-3.10320571

f-Ag₆...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600

C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-1.81620429	-1.88370571	-1.00943529
Ag	1.12679059	1.23164114	-2.64148670
Ag	2.52977445	-1.21010640	-2.31708023
Ag	0.70916422	-3.13631707	-1.30823540
Ag	-1.55780674	0.81449609	-1.83622844
Ag	-0.09921265	-1.16303819	-2.98185434

g-Ag₆...Coronene

C	2.97875278	3.44431539	0.16995756
C	3.30135402	2.08833567	0.49691309
C	2.25397081	1.19238429	0.83029036
C	3.89528912	-0.62999212	1.11798636
C	2.55179610	-0.17364221	1.14334838

C	4.16763358	-2.00452377	1.41471703
C	1.78520590	-2.44086385	1.75064182
C	0.70839585	-3.33829732	2.04293562
C	1.49228846	-1.08285366	1.46660091
C	-0.59756774	-2.90309470	2.03483025
H	0.94094137	-4.37660233	2.26132421
C	0.13414710	-0.62945784	1.46150680
C	-0.91755578	-1.54005515	1.73631489
H	-1.40870004	-3.59374740	2.24698337
C	-0.16447166	0.73330738	1.13499834
C	-2.27098105	-1.07436036	1.68722983
C	-1.51360759	1.17224710	1.08785407
C	0.89586152	1.64542147	0.82384981
C	-2.55940433	0.23550239	1.37341706
H	-3.07100449	-1.77851883	1.89733817
C	-1.79001330	2.53461593	0.74265404
C	0.59813689	2.98877977	0.48197206
H	-3.58972718	0.57779853	1.33355228
C	-0.76950598	3.41253793	0.45256831
H	-2.82514764	2.86277517	0.70979178
H	-0.98944138	4.44313286	0.18909326
C	3.14839224	-2.87919675	1.71961781
C	1.67257796	3.87939527	0.16208953
C	4.93735354	0.29428812	0.78447808
C	4.65019997	1.60750503	0.48561979
H	3.36462056	-3.92120165	1.93745199
H	1.43650582	4.90781077	-0.09578702
H	3.78680969	4.12542346	-0.08138877
H	5.44706809	2.30019138	0.23011606
H	5.96358718	-0.06199664	0.76821069

H	5.19840543	-2.34705185	1.39131816
Ag	2.77492950	-0.05991976	-3.24893733
Ag	-1.57809108	-1.17750031	-2.33656552
Ag	0.04721132	-3.41550086	-1.71569516
Ag	2.73901890	-2.72357810	-2.27969150
Ag	0.10719998	0.89550722	-3.28099528
Ag	0.95360029	-0.87734109	-1.41251658

h-Ag₆...Coronene

C	0.15518657	4.33031870	3.49439413
C	0.81271408	3.05858500	3.49253328
C	0.04848650	1.88778518	3.72931338
C	2.07494211	0.50250287	3.46057338
C	0.68230707	0.60295912	3.71424279
C	2.68368228	-0.79367552	3.43032745
C	0.53092637	-1.85466338	3.89845831
C	-0.26734094	-3.02656140	4.09787427
C	-0.09216768	-0.58158191	3.93955481
C	-1.62399499	-2.93090626	4.31082452
H	0.21752276	-3.99804962	4.06679187
C	-1.50271639	-0.48194931	4.16442667
C	-2.27641483	-1.65702120	4.34157822
H	-2.22325172	-3.82613331	4.45012848
C	-2.13854296	0.80204160	4.16580572
C	-3.69153261	-1.53646431	4.52582979
C	-3.54334620	0.89782311	4.34583953
C	-1.36214839	1.98733088	3.95279687
C	-4.30402071	-0.30266408	4.52731271
H	-4.27739716	-2.44145122	4.65918493
C	-4.16038390	2.19030644	4.32677821
C	-1.99507551	3.25588093	3.93502347

H	-5.37897891	-0.22206718	4.66255326
C	-3.41179945	3.32942229	4.13089979
H	-5.23584801	2.25498235	4.46629702
H	-3.88936960	4.30492168	4.11527070
C	1.93776104	-1.93210206	3.64117506
C	-1.20160958	4.42576173	3.70756982
C	2.82777913	1.69899244	3.23020606
C	2.21795500	2.93355744	3.24681569
H	2.40762140	-2.91101117	3.61037192
H	-1.69344776	5.39420476	3.69850721
H	0.74787100	5.22288551	3.31526061
H	2.79669138	3.83516576	3.06719953
H	3.89369893	1.61435927	3.03782324
H	3.74990939	-0.86279304	3.23348710
Ag	-2.98593228	-0.71171613	-1.84456774
Ag	-1.88912799	-2.13806372	0.58462178
Ag	-3.30892597	0.09986636	1.15025651
Ag	-0.98954201	0.18895547	-0.24853623
Ag	0.14845956	2.15765042	0.47913115
Ag	-2.48522885	2.34027845	-0.13277765

i-Ag₆...Coronene

C	2.05603600	-1.29315300	-3.11952000
C	1.43734400	-0.02338500	-2.88514600
C	0.10386800	0.01644000	-2.40431700
C	0.17596500	2.48406600	-2.36853300
C	-0.52832100	1.27575800	-2.14060400
C	-0.46983600	3.72944700	-2.08238500
C	-2.48212400	2.55708900	-1.33940600
C	-3.80677600	2.56961300	-0.79554700
C	-1.86709000	1.31293800	-1.63067000

C	-4.48400300	1.39619400	-0.55500500
H	-4.26749900	3.52714900	-0.57018200
C	-2.57029900	0.09206100	-1.37838700
C	-3.88352700	0.12943500	-0.84110500
H	-5.48661000	1.41482300	-0.13741900
C	-1.94347200	-1.16505000	-1.65794700
C	-4.56181500	-1.10091800	-0.58095700
C	-2.63184600	-2.37000700	-1.38455400
C	-0.59966100	-1.20392000	-2.14976700
C	-3.95640200	-2.30804800	-0.84086900
H	-5.56455500	-1.06655500	-0.16385100
C	-1.97094200	-3.61933500	-1.61637300
C	0.03644500	-2.45217300	-2.37880200
H	-4.47602800	-3.23946100	-0.63547000
C	-0.68074900	-3.65952800	-2.09559800
H	-2.50377100	-4.53943100	-1.39351000
H	-0.18333100	-4.61114200	-2.25945300
C	-1.75382700	3.76437200	-1.58287600
C	1.37971500	-2.46737200	-2.87253700
C	1.52527600	2.42070100	-2.84441500
C	2.13520400	1.20943400	-3.09273400
H	-2.23199200	4.71433500	-1.36112100
H	1.86274800	-3.42613200	-3.03729500
H	3.07953400	-1.31345000	-3.48238800
H	3.16185100	1.17268800	-3.44572400
H	2.06452600	3.34999400	-3.00390000
H	0.07695900	4.65154100	-2.25784600
Ag	2.01696000	1.07248500	0.43937600
Ag	0.28120600	3.24187700	1.28223800
Ag	3.59052400	-1.32276500	0.24574200

Ag	-0.79915600	0.61458900	1.52211300
Ag	-1.88218200	-2.01918000	1.76258000
Ag	0.84612000	-1.76577900	0.90915200

j-Ag₆...Coronene

C	0.23630910	4.34712187	3.63112278
C	0.89383661	3.07538817	3.62926193
C	0.12960903	1.90458835	3.86604203
C	2.15606464	0.51930604	3.59730203
C	0.76342960	0.61976229	3.85097144
C	2.76480481	-0.77687235	3.56705610
C	0.61204890	-1.83786021	4.03518696
C	-0.18621841	-3.00975823	4.23460292
C	-0.01104515	-0.56477874	4.07628346
C	-1.54287246	-2.91410309	4.44755317
H	0.29864529	-3.98124645	4.20352052
C	-1.42159386	-0.46514614	4.30115532
C	-2.19529230	-1.64021803	4.47830687
H	-2.14212919	-3.80933014	4.58685713
C	-2.05742043	0.81884477	4.30253437
C	-3.61041008	-1.51966114	4.66255844
C	-3.46222367	0.91462628	4.48256818
C	-1.28102586	2.00413405	4.08952552
C	-4.22289818	-0.28586091	4.66404136
H	-4.19627463	-2.42464805	4.79591358
C	-4.07926137	2.20710961	4.46350686
C	-1.91395298	3.27268410	4.07175212
H	-5.29785638	-0.20526401	4.79928191
C	-3.33067692	3.34622546	4.26762844
H	-5.15472548	2.27178552	4.60302567
H	-3.80824707	4.32172485	4.25199935

C	2.01888357	-1.91529889	3.77790371
C	-1.12048705	4.44256490	3.84429847
C	2.90890166	1.71579561	3.36693471
C	2.29907753	2.95036061	3.38354434
H	2.48874393	-2.89420800	3.74710057
H	-1.61232523	5.41100793	3.83523586
H	0.82899353	5.23968868	3.45198926
H	2.87781391	3.85196893	3.20392818
H	3.97482146	1.63116244	3.17455189
H	3.83103192	-0.84598987	3.37021575
Ag	-2.45930283	0.83788115	1.56812438
Ag	-0.47562887	-1.43202531	1.34235670
Ag	0.60639944	1.03215540	1.02435010
Ag	-1.22487622	0.03625428	-0.70732839
Ag	-0.54364811	0.75609162	-2.87944018
Ag	-0.57385133	2.57181282	-0.86788748

a-Ag₇...Coronene

C	0.86050337	3.62672263	-0.62019956
C	1.57341802	2.65459713	0.15205507
C	0.87068295	1.53808318	0.67209437
C	2.96129123	0.67546220	1.66355424
C	1.56734734	0.54351587	1.43250757
C	3.64099728	-0.34112539	2.40928020
C	1.55542080	-1.58941515	2.67638169
C	0.83456435	-2.72996861	3.15580444
C	0.86030070	-0.59217880	1.94631372
C	-0.51090192	-2.87431565	2.90303507
H	1.37363158	-3.48866644	3.71583338
C	-0.53987498	-0.74069892	1.68633003
C	-1.22963023	-1.88738022	2.15552676

H	-1.04707801	-3.74843340	3.26133533
C	-1.23341380	0.24710961	0.91422369
C	-2.62110523	-2.03494431	1.85046431
C	-2.61181593	0.07833077	0.61997940
C	-0.52906661	1.38890299	0.41095947
C	-3.28899982	-1.08603706	1.10823878
H	-3.14191637	-2.91699043	2.21208921
C	-3.28120924	1.06972085	-0.16784692
C	-1.21179593	2.35596632	-0.36929758
H	-4.34342869	-1.20975277	0.87759795
C	-2.60521337	2.17118420	-0.64338877
H	-4.33638346	0.93354938	-0.38770186
H	-3.12101804	2.91617313	-1.24243269
C	2.96203892	-1.43528782	2.89784375
C	-0.48515927	3.48224651	-0.87272237
C	3.64909101	1.81463958	1.13381247
C	2.97817198	2.77097853	0.40470646
H	3.48764608	-2.20391909	3.45723960
H	-1.01603056	4.22034569	-1.46707421
H	1.40510527	4.48080345	-1.01262009
H	3.50926229	3.62961445	0.00372920
H	4.71598882	1.90950550	1.31571483
H	4.70855246	-0.23428089	2.58037604
Ag	0.54812712	-0.68514169	-1.29842942
Ag	0.52881699	-2.99600486	-3.16350112
Ag	2.53689364	-2.67285870	-1.22168818
Ag	-0.31062628	-0.43370020	-3.96488412
Ag	-0.08831787	-3.28486400	-0.43391835
Ag	-1.84845881	-1.90340259	-2.13055089
Ag	2.39945477	-0.90875853	-3.40220403

b-Ag7...Coronene

C	0.00871310	3.82335877	-0.45265997
C	0.77077079	2.87658754	0.30400694
C	0.11542924	1.74335629	0.84916311
C	2.25704354	0.94689519	1.78558638
C	0.86156630	0.77361768	1.59456245
C	2.98646054	-0.04542619	2.51689135
C	0.94611690	-1.35157161	2.84882775
C	0.27222497	-2.50958684	3.35401364
C	0.20229608	-0.37894586	2.13370450
C	-1.07506440	-2.69399186	3.13997145
H	0.84846414	-3.24924078	3.90238281
C	-1.19973998	-0.56913587	1.91401306
C	-1.84266544	-1.73244152	2.40813118
H	-1.57551596	-3.58107686	3.51756137
C	-1.94288641	0.39386929	1.15687079
C	-3.23729862	-1.92168567	2.14312955
C	-3.32354136	0.18385751	0.90241964
C	-1.28619423	1.55251210	0.62831220
C	-3.95286059	-0.99665596	1.41532600
H	-3.72207550	-2.81623494	2.52364912
C	-4.04310579	1.15104594	0.12886577
C	-2.01816905	2.49504463	-0.13717926
H	-5.00932424	-1.15194774	1.21510108
C	-3.41280016	2.26872110	-0.37098323
H	-5.09965215	0.98334449	-0.06049499
H	-3.96649285	2.99511567	-0.95893895
C	2.35334880	-1.15581366	3.02980403
C	-1.33876184	3.63882050	-0.66644952
C	2.89653536	2.10229504	1.23104026

C	2.17810434	3.03474194	0.51639926
H	2.91640802	-1.90578721	3.57796882
H	-1.90717844	4.35792236	-1.24925645
H	0.51720637	4.69046094	-0.86449436
H	2.67272562	3.90595968	0.09636978
H	3.96492553	2.22882686	1.38233824
H	4.05485872	0.09303567	2.65730938
Ag	0.46151733	-0.80888373	-3.23703111
Ag	0.66946130	-3.48200440	-1.96026210
Ag	1.54777202	-1.14604168	-0.66439128
Ag	1.04572339	-3.12324469	-4.72467943
Ag	-1.19613311	-1.56284018	-1.09349609
Ag	-1.50674176	-2.78710819	-3.60144023
Ag	2.93302061	-2.10803276	-2.90966358

c-Ag₇...Coronene

C	0.57091261	4.07128898	-0.25418092
C	1.29200641	2.90617376	0.16076817
C	0.60837600	1.89275961	0.87946288
C	2.68023707	0.55251459	0.97372636
C	1.30560491	0.71004053	1.28907375
C	3.35200377	-0.64696167	1.37565180
C	1.29577201	-1.50244522	2.38523520
C	0.57565680	-2.53161746	3.07268045
C	0.61167414	-0.32063106	2.00313975
C	-0.76575241	-2.39300047	3.34911229
H	1.10705603	-3.43314934	3.36371896
C	-0.78278938	-0.17504641	2.29368797
C	-1.47983403	-1.21495880	2.95964358
H	-1.30626685	-3.18384628	3.86131612
C	-1.48293798	1.00172714	1.87189900

C	-2.88280139	-1.06529008	3.20525055
C	-2.87463753	1.12707686	2.12193549
C	-0.78626668	2.03774189	1.16876707
C	-3.55708024	0.06550968	2.80022359
H	-3.40988614	-1.86711659	3.71444412
C	-3.55795231	2.30448070	1.67649962
C	-1.48407264	3.19309355	0.73476102
H	-4.62256958	0.16725444	2.98650690
C	-2.88537236	3.30349824	1.00871810
H	-4.62281499	2.39305820	1.87269592
H	-3.41300695	4.19141571	0.67238362
C	2.68309583	-1.63967597	2.05679108
C	-0.77061123	4.20979065	0.02255020
C	3.35163485	1.59189371	0.25238313
C	2.68103593	2.72912566	-0.13916851
H	3.19995558	-2.54831177	2.35211737
H	-1.31162873	5.09331273	-0.30388146
H	1.10221158	4.84460880	-0.80166336
H	3.19793565	3.51033958	-0.68927288
H	4.40430368	1.46480986	0.01553513
H	4.40385659	-0.76132549	1.12889248
Ag	-0.51702800	-0.60775503	-0.91715634
Ag	-1.11305974	-1.99977464	-3.47175641
Ag	1.08296301	-2.71664563	-1.86831859
Ag	-1.54757069	0.76042059	-3.14801674
Ag	-1.52995919	-3.23100110	-0.97672266
Ag	-3.15653091	-1.08374735	-1.76960315
Ag	1.07254243	-0.24866180	-3.20792130

d-Ag7...Coronene

C	-5.69455117	2.87401061	1.18382553
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C	-4.37228615	3.42486103	1.22184187
C	-3.26044437	2.54516597	1.23934442
C	-1.72561685	4.47670773	1.21128970
C	-1.92953935	3.07399979	1.23492856
C	-0.38720120	4.98460626	1.16210915
C	0.51135664	2.71055463	1.18639133
C	1.61946659	1.80559064	1.13409561
C	-0.80509254	2.18577200	1.22421034
C	1.42101973	0.44093190	1.13069368
H	2.62481470	2.21498815	1.09329744
C	-1.01253005	0.76789857	1.21526407
C	0.09952094	-0.11116124	1.17697292
H	2.26941207	-0.23666603	1.09204140
C	-2.34340089	0.23877493	1.22335069
C	-0.12957276	-1.52350271	1.15647911
C	-2.54732157	-1.16394662	1.19121659
C	-3.46798639	1.12728052	1.23391461
C	-1.40965468	-2.03261439	1.16350131
H	0.72882084	-2.18806264	1.12384104
C	-3.88631493	-1.67150804	1.15751108
C	-4.78529717	0.60322309	1.20824697
H	-1.57479246	-3.10603833	1.13867632
C	-4.96842187	-0.81635292	1.16490885
H	-4.03597709	-2.74709834	1.12518659
H	-5.98010572	-1.21024440	1.13143595
C	0.69436951	4.12964186	1.15246867
C	-5.89367350	1.50956678	1.17686314
C	-2.86262615	5.34589871	1.20321893
C	-4.14280953	4.83746112	1.21087473
H	1.70633736	4.52192999	1.10898810

H	-6.89924896	1.10021704	1.14192383
H	-6.54184462	3.55367467	1.15945840
H	-5.00048663	5.50341731	1.19327233
H	-2.69725558	6.41921025	1.18014821
H	-0.23834002	6.06014347	1.13289003
Ag	-0.06997918	0.13293346	-2.78298184
Ag	0.37977482	2.95242846	-2.76882384
Ag	-1.87542918	4.88678146	-2.57280384
Ag	-4.65896018	3.77271546	-2.77688184
Ag	-5.10864518	0.95311346	-2.77492484
Ag	-2.85233018	-0.97850854	-2.56677884
Ag	-2.36390218	1.95410046	-2.56972984

f-Ag7...Coronene

C	-3.35678000	1.60908600	2.29876800
C	-1.97879700	2.00093700	2.32846400
C	-0.97782700	0.99681700	2.34126900
C	0.77294400	2.73478800	2.30134600
C	0.40590800	1.36574500	2.32852300
C	2.16142300	3.08199700	2.24383000
C	2.78694400	0.71820900	2.26699100
C	3.78084100	-0.31064000	2.21006300
C	1.41823200	0.35164200	2.31305200
C	3.42355400	-1.64256800	2.21010400
H	4.82704600	-0.02214100	2.16295600
C	1.04573800	-1.03208300	2.30769000
C	2.04667000	-2.03565500	2.26470000
H	4.18630200	-2.41511900	2.16787900
C	-0.33797600	-1.40129900	2.32410700
C	1.65325300	-3.41135600	2.24790200
C	-0.70533200	-2.77041400	2.29551200

C	-1.35040600	-0.38690400	2.33942400
C	0.32231900	-3.76666200	2.26293700
H	2.42749800	-4.17212700	2.21161300
C	-2.09482100	-3.11730700	2.27014600
C	-2.72025300	-0.75271600	2.32200300
H	0.03217500	-4.81330200	2.24087100
C	-3.06900000	-2.14102200	2.28211700
H	-2.36989400	-4.16792300	2.24049800
H	-4.12010300	-2.41345600	2.25496300
C	3.13507900	2.10596200	2.22961900
C	-3.71473300	0.27744700	2.29525200
C	-0.25419800	3.73144100	2.29813100
C	-1.58515000	3.37681700	2.31379900
H	4.18583400	2.37669000	2.17982200
H	-4.76159300	-0.01105700	2.26662400
H	-4.11855600	2.38349400	2.27796500
H	-2.35880800	4.13883800	2.29984200
H	0.03588900	4.77789200	2.27230100
H	2.43534100	4.13259000	2.21194000
Ag	2.07531100	2.06547500	-1.02600800
Ag	2.82211600	-0.69530400	-1.01459100
Ag	0.78454300	-2.86249100	-1.16142900
Ag	-2.10528500	-2.04937900	-1.02125700
Ag	-2.85395200	0.71240800	-0.96546200
Ag	-0.81826100	2.87802100	-1.12672000
Ag	-0.01610800	0.00897200	-1.26244300

a-Ag₈...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300

C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900

H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-1.29759440	2.20905671	-2.37046926
Ag	-3.80230688	0.88155494	-2.03695639
Ag	-3.82662898	-1.81153266	-1.88853602
Ag	-1.34655794	-3.21252615	-2.07169241
Ag	1.06369340	-1.89925647	-2.39493187
Ag	1.08829596	0.82503586	-2.54506570
Ag	-1.39741851	-0.50062823	-2.21334966
Ag	3.43658247	-0.57193436	-2.71506946

b-Ag₈...Coronene

C	2.39230761	4.35460964	0.07335250
C	2.94511427	3.05924145	0.33041001
C	2.07665894	2.00063054	0.69920416
C	3.99892367	0.45490508	0.81488362
C	2.60565837	0.69176223	0.94365659
C	4.50301067	-0.86599333	1.04440821
C	2.24751177	-1.68262455	1.51878986
C	1.34743038	-2.74634668	1.84847320
C	1.72662626	-0.38160844	1.30267201
C	-0.00788629	-2.52358649	1.94068238
H	1.75423327	-3.73974422	2.01436787
C	0.31726666	-0.14923577	1.40191974
C	-0.55723890	-1.22153908	1.71206728
H	-0.68416272	-3.33911193	2.18050343
C	-0.21294258	1.15662039	1.14398981
C	-1.96694550	-0.97519121	1.76757391
C	-1.61410158	1.37719163	1.20020536
C	0.66729312	2.23268760	0.79709435

C	-2.47794684	0.27974976	1.51976819
H	-2.63030675	-1.80223609	2.00415540
C	-2.12366814	2.68663976	0.92217745
C	0.13992909	3.51991004	0.52309171
H	-3.54937667	0.45528363	1.55909983
C	-1.27585020	3.72212409	0.59766408
H	-3.19713787	2.84728401	0.96830431
H	-1.67216844	4.71102529	0.38571396
C	3.65696519	-1.89843645	1.38372880
C	1.03681860	4.57720933	0.16580775
C	4.85769718	1.54063811	0.44730804
C	4.34846526	2.79872120	0.21445207
H	4.04823233	-2.89805866	1.54999999
H	0.62533376	5.56126307	-0.03958770
H	3.06431326	5.16119593	-0.20569250
H	5.00734588	3.61506511	-0.06760161
H	5.92337101	1.35203688	0.35176842
H	5.57050563	-1.04012035	0.94194907
Ag	0.27276179	-0.99458023	-1.68453170
Ag	-0.45881757	-2.82809943	-3.74610279
Ag	-0.52667453	-1.94607230	-6.29419317
Ag	0.13614178	0.78107599	-6.81421061
Ag	0.84060733	2.53353650	-4.79651813
Ag	0.90925584	1.64128608	-2.21890475
Ag	0.18330388	-0.17565698	-4.27265957
Ag	1.53489124	4.24729361	-2.77763700

c-Ag...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300

C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100
C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900

H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	1.04955647	-1.10380874	-3.23217515
Ag	-1.18388396	-1.70430384	-1.58126918
Ag	-1.12707116	-4.05030443	-3.18357830
Ag	-0.75176677	-2.08319223	-5.19950420
Ag	1.36694000	-3.63518046	-4.40296978
Ag	-1.33707986	0.18447493	-3.65210981
Ag	-3.06660904	-2.15678464	-3.61349519
Ag	1.02358348	-3.33411907	-1.52795204

d-Ag₈...Coronene

C	0.94799182	3.92085614	-0.04415641
C	1.63270082	2.68609914	0.19291159
C	0.87965482	1.53809114	0.54770759
C	2.95190282	0.19812414	0.63730259
C	1.54203982	0.28762514	0.77201659
C	3.59070482	-1.06666986	0.84655359
C	1.43337782	-2.11910486	1.31294459
C	0.64927582	-3.27490686	1.62861559
C	0.77996882	-0.87601586	1.11683759
C	-0.72150418	-3.19497186	1.72649559
H	1.15722182	-4.22314686	1.77921459
C	-0.64553518	-0.79221586	1.22199259
C	-1.40337518	-1.95362386	1.51795859
H	-1.30897918	-4.07947886	1.95555059
C	-1.30885618	0.45532314	0.98416559
C	-2.83081418	-1.85533186	1.57958259
C	-2.72512418	0.52885414	1.04610559
C	-0.54582718	1.62159614	0.65150059

C	-3.46972918	-0.65658686	1.35109859
H	-3.40426218	-2.74991186	1.80520659
C	-3.36835118	1.78239114	0.78819859
C	-1.20444318	2.85112914	0.39732459
H	-4.55343518	-0.59347586	1.39490859
C	-2.63329318	2.90462614	0.47737659
H	-4.45252318	1.83038514	0.83858859
H	-3.13049718	3.85014214	0.28064259
C	2.85714382	-2.18590986	1.17222259
C	-0.42294218	4.00061014	0.05396759
C	3.69251682	1.37208614	0.28413959
C	3.05508582	2.57392414	0.07064659
H	3.35028282	-3.14195386	1.32313459
H	-0.93470818	4.93964114	-0.13625641
H	1.53201482	4.79659514	-0.31255441
H	3.62503482	3.45805214	-0.20059341
H	4.77166482	1.29619214	0.18394659
H	4.67014382	-1.12788086	0.73965059
Ag	0.87728735	0.17433666	-2.35612501
Ag	-1.68004791	-0.94810711	-1.83220007
Ag	-0.96670933	-2.43792659	-4.14432614
Ag	-0.18965522	0.16127389	-4.98971646
Ag	1.72972985	-1.67178150	-4.29120245
Ag	-1.38455416	1.62516282	-2.91400432
Ag	-2.84977771	-0.45051859	-4.33489323
Ag	0.54547691	-2.55328589	-1.78226768

f-Ag₈...Coronene

C	0.57673487	3.62926848	1.03435755
C	1.26144387	2.39451148	1.27142555
C	0.50839787	1.24650348	1.62622155

C	2.58064587	-0.09346352	1.71581655
C	1.17078287	-0.00396252	1.85053055
C	3.21944787	-1.35825752	1.92506755
C	1.06212087	-2.41069252	2.39145855
C	0.27801887	-3.56649452	2.70712955
C	0.40871187	-1.16760352	2.19535155
C	-1.09276113	-3.48655952	2.80500955
H	0.78596487	-4.51473452	2.85772855
C	-1.01679213	-1.08380352	2.30050655
C	-1.77463213	-2.24521152	2.59647255
H	-1.68023613	-4.37106652	3.03406455
C	-1.68011313	0.16373548	2.06267955
C	-3.20207113	-2.14691952	2.65809655
C	-3.09638113	0.23726648	2.12461955
C	-0.91708413	1.33000848	1.73001455
C	-3.84098613	-0.94817452	2.42961255
H	-3.77551913	-3.04149952	2.88372055
C	-3.73960813	1.49080348	1.86671255
C	-1.57570013	2.55954148	1.47583855
H	-4.92469213	-0.88506352	2.47342255
C	-3.00455013	2.61303848	1.55589055
H	-4.82378013	1.53879748	1.91710255
H	-3.50175413	3.55855448	1.35915655
C	2.48588687	-2.47749752	2.25073655
C	-0.79419913	3.70902248	1.13248155
C	3.32125987	1.08049848	1.36265355
C	2.68382887	2.28233648	1.14916055
H	2.97902587	-3.43354152	2.40164855
H	-1.30596513	4.64805348	0.94225755
H	1.16075787	4.50500748	0.76595955

H	3.25377787	3.16646448	0.87792055
H	4.40040787	1.00460448	1.26246055
H	4.29888687	-1.41946852	1.81816455
Ag	1.14871189	-0.27746287	-4.21167082
Ag	0.30221580	-0.98388384	-1.59274837
Ag	-1.79788324	-2.15383571	-3.10771954
Ag	-1.61216956	0.36475927	-4.41022895
Ag	-0.64632595	-1.88333427	-5.65331966
Ag	0.07685581	1.63940734	-2.56583182
Ag	-2.26448279	0.14845798	-1.68864184
Ag	0.87482782	-2.95495422	-3.41457435

a-Ag₉...Coronene

C	-2.80411100	1.21010800	-3.79779400
C	-2.54964100	2.09781800	-2.70198400
C	-2.93620800	1.70682300	-1.39358600
C	-1.97322100	3.78863300	-0.48224100
C	-2.64242400	2.55525200	-0.27774500
C	-1.64713300	4.60101400	0.65264500
C	-2.62958700	2.94734100	2.16057700
C	-2.92993500	2.48480900	3.48199400
C	-2.97077600	2.13251700	1.05041300
C	-3.52381400	1.25958000	3.68669100
H	-2.66690400	3.11515800	4.32638300
C	-3.57719500	0.85047100	1.26394500
C	-3.85688300	0.40872300	2.58362900
H	-3.73625500	0.91231300	4.69362200
C	-3.87764400	0.00380500	0.14638200
C	-4.43648900	-0.88754400	2.77483600
C	-4.43524400	-1.28274700	0.36258600
C	-3.54697200	0.42788600	-1.18148800

C	-4.71458800	-1.70462800	1.70219600
H	-4.64208300	-1.22068900	3.78799800
C	-4.67423500	-2.13551100	-0.76345300
C	-3.78607800	-0.43596100	-2.28137300
H	-5.14094200	-2.69156400	1.85800000
C	-4.36082300	-1.72562600	-2.04180300
H	-5.10439700	-3.11812600	-0.59091700
H	-4.53757600	-2.38270300	-2.88855200
C	-1.96742800	4.19517700	1.92955400
C	-3.40435400	-0.01287000	-3.59480200
C	-1.61136600	4.17249900	-1.81410800
C	-1.88995400	3.35537200	-2.88665000
H	-1.70752200	4.81232800	2.78481300
H	-3.58259500	-0.68374300	-4.43016000
H	-2.50429000	1.51670500	-4.79570000
H	-1.59913000	3.64759400	-3.89152700
H	-1.10019700	5.11959700	-1.96194100
H	-1.13550800	5.54504200	0.48712700
Ag	-1.26441100	-2.55997300	-0.57263100
Ag	0.77523000	-2.80731200	1.71893500
Ag	-0.64058900	-0.22083300	1.29149400
Ag	1.73934000	-2.34972100	-1.05158600
Ag	-0.08389600	-0.05198800	-1.77020000
Ag	2.40923800	-0.44139700	1.32995200
Ag	0.89337500	1.99430000	0.19974600
Ag	2.89059000	0.25597100	-1.56340600
Ag	3.87546300	2.03947200	0.61238500

b-Ag₉...Coronene

C	6.51140178	-0.01233521	-1.74708150
C	6.34331269	0.13243299	-0.33132312

C	5.58477435	-0.83651577	0.37576553
C	6.06743733	0.32783957	2.49782577
C	5.44999755	-0.74005287	1.79835896
C	5.95945170	0.38007516	3.92606702
C	4.65626950	-1.68760892	3.93645299
C	3.97972575	-2.73398496	4.64191269
C	4.74223056	-1.75305326	2.52183646
C	3.43288319	-3.80407132	3.96985790
H	3.91698231	-2.67568953	5.72458662
C	4.18441705	-2.87420343	1.82265963
C	3.52659834	-3.90459800	2.54411240
H	2.93253855	-4.59899889	4.51518441
C	4.31333029	-2.96748407	0.39761925
C	3.00219985	-5.02924615	1.82788331
C	3.80109789	-4.09964537	-0.28700235
C	5.02311004	-1.95377516	-0.32420784
C	3.13593117	-5.12375528	0.46087715
H	2.50541103	-5.81633832	2.38773910
C	3.99120949	-4.20094704	-1.70329417
C	5.20546704	-2.07810776	-1.72579183
H	2.74751914	-5.98715863	-0.07181979
C	4.66975581	-3.22308967	-2.39883811
H	3.59356195	-5.06901346	-2.22163516
H	4.81654608	-3.31296615	-3.47138205
C	5.27459671	-0.59279355	4.62053751
C	5.95894286	-1.07887237	-2.42121816
C	6.81059421	1.30600496	1.76089146
C	6.94383479	1.21146645	0.39379104
H	5.20628268	-0.55095172	5.70380889
H	6.10158210	-1.18617459	-3.49257417

H	7.09410165	0.73315727	-2.28038494
H	7.52120004	1.94955351	-0.15541470
H	7.27922009	2.12153232	2.30444263
H	6.43436820	1.20221891	4.45415715
Ag	-1.26441100	-2.55997300	-0.57263100
Ag	0.77523000	-2.80731200	1.71893500
Ag	-0.64058900	-0.22083300	1.29149400
Ag	1.73934000	-2.34972100	-1.05158600
Ag	-0.08389600	-0.05198800	-1.77020000
Ag	2.40923800	-0.44139700	1.32995200
Ag	0.89337500	1.99430000	0.19974600
Ag	2.89059000	0.25597100	-1.56340600
Ag	3.87546300	2.03947200	0.61238500

c-Ag₉...Coronene

C	0.98451229	3.81327206	-0.14794264
C	1.65086248	2.56370412	0.06231882
C	0.92735116	1.48434813	0.63012414
C	2.92819630	0.04674903	0.46375659
C	1.56887248	0.21941739	0.83293995
C	3.54329964	-1.23226248	0.65697995
C	1.46211681	-2.13480297	1.56983178
C	0.70085101	-3.22301179	2.10519926
C	0.83410626	-0.87573135	1.39372686
C	-0.62691008	-3.06449040	2.43219980
H	1.18944356	-4.18387403	2.23887563
C	-0.54604075	-0.70997597	1.73703585
C	-1.28517521	-1.80652113	2.24894877
H	-1.19932493	-3.89880239	2.82743446
C	-1.19098310	0.55114781	1.52133659
C	-2.67433027	-1.62925529	2.54872531

C	-2.57007600	0.70318153	1.82141485
C	-0.45302614	1.64971373	0.97211496
C	-3.29555287	-0.41737312	2.34176886
H	-3.23395336	-2.47457819	2.93894752
C	-3.19856003	1.96782702	1.58205819
C	-1.09693798	2.89151542	0.74094838
H	-4.35117444	-0.29446856	2.56733167
C	-2.48600393	3.02551298	1.06254284
H	-4.25407783	2.07615437	1.81533668
H	-2.97227750	3.97988750	0.88192203
C	2.83495346	-2.28601079	1.19058131
C	-0.34336439	3.97163821	0.17933817
C	3.64079627	1.15272748	-0.10231137
C	3.02380009	2.36865564	-0.29504578
H	3.30872919	-3.25384691	1.32773250
H	-0.84306845	4.92077103	0.00813190
H	1.54624478	4.63629422	-0.58052823
H	3.57152135	3.20057722	-0.72863915
H	4.68148288	1.01340621	-0.38145272
H	4.58367025	-1.35743875	0.37005925
Ag	-3.04781063	-1.62361410	-2.46567753
Ag	1.30651337	-1.75925810	-2.45930353
Ag	-2.95975163	0.05941990	-4.79127253
Ag	1.56822137	-0.13942310	-4.73053153
Ag	-3.25585763	-2.80175110	-4.98296153
Ag	1.25565637	-2.97553010	-5.05254453
Ag	-0.77148863	-0.12813410	-3.15619453
Ag	-0.94697663	-3.10928810	-3.41772453
Ag	-0.84582463	-1.38337510	-5.74854853

d-Ag₉...Coronene

C	0.98451229	3.81327206	-0.14794264
C	1.65086248	2.56370412	0.06231882
C	0.92735116	1.48434813	0.63012414
C	2.92819630	0.04674903	0.46375659
C	1.56887248	0.21941739	0.83293995
C	3.54329964	-1.23226248	0.65697995
C	1.46211681	-2.13480297	1.56983178
C	0.70085101	-3.22301179	2.10519926
C	0.83410626	-0.87573135	1.39372686
C	-0.62691008	-3.06449040	2.43219980
H	1.18944356	-4.18387403	2.23887563
C	-0.54604075	-0.70997597	1.73703585
C	-1.28517521	-1.80652113	2.24894877
H	-1.19932493	-3.89880239	2.82743446
C	-1.19098310	0.55114781	1.52133659
C	-2.67433027	-1.62925529	2.54872531
C	-2.57007600	0.70318153	1.82141485
C	-0.45302614	1.64971373	0.97211496
C	-3.29555287	-0.41737312	2.34176886
H	-3.23395336	-2.47457819	2.93894752
C	-3.19856003	1.96782702	1.58205819
C	-1.09693798	2.89151542	0.74094838
H	-4.35117444	-0.29446856	2.56733167
C	-2.48600393	3.02551298	1.06254284
H	-4.25407783	2.07615437	1.81533668
H	-2.97227750	3.97988750	0.88192203
C	2.83495346	-2.28601079	1.19058131
C	-0.34336439	3.97163821	0.17933817
C	3.64079627	1.15272748	-0.10231137
C	3.02380009	2.36865564	-0.29504578

H	3.30872919	-3.25384691	1.32773250
H	-0.84306845	4.92077103	0.00813190
H	1.54624478	4.63629422	-0.58052823
H	3.57152135	3.20057722	-0.72863915
H	4.68148288	1.01340621	-0.38145272
H	4.58367025	-1.35743875	0.37005925
Ag	-1.53119409	-0.99602778	-2.12446977
Ag	-1.24384853	1.69408032	-2.69571602
Ag	-3.65111913	0.70261739	-1.69609435
Ag	-3.88969614	-2.01568735	-1.13661479
Ag	-1.70872908	-3.68794200	-1.59055757
Ag	0.66193850	-2.61374196	-2.59216801
Ag	0.99855256	0.09766657	-3.18405029
Ag	3.02285549	-1.69395054	-3.56330157
Ag	1.04211669	2.78329199	-3.67092197

f-Ag₉...Coronene

C	0.89951707	3.66542850	1.06408091
C	1.56586726	2.41586056	1.27434237
C	0.84235594	1.33650457	1.84214769
C	2.84320108	-0.10109453	1.67578014
C	1.48387726	0.07157383	2.04496350
C	3.45830442	-1.38010604	1.86900350
C	1.37712159	-2.28264653	2.78185533
C	0.61585579	-3.37085535	3.31722281
C	0.74911104	-1.02357491	2.60575041
C	-0.71190530	-3.21233396	3.64422335
H	1.10444834	-4.33171759	3.45089918
C	-0.63103597	-0.85781953	2.94905940
C	-1.37017043	-1.95436469	3.46097232
H	-1.28432015	-4.04664595	4.03945801

C	-1.27597832	0.40330425	2.73336014
C	-2.75932549	-1.77709885	3.76074886
C	-2.65507122	0.55533797	3.03343840
C	-0.53802136	1.50187017	2.18413851
C	-3.38054809	-0.56521668	3.55379241
H	-3.31894858	-2.62242175	4.15097107
C	-3.28355525	1.81998346	2.79408174
C	-1.18193320	2.74367186	1.95297193
H	-4.43616966	-0.44231212	3.77935522
C	-2.57099915	2.87766942	2.27456639
H	-4.33907305	1.92831081	3.02736023
H	-3.05727272	3.83204394	2.09394558
C	2.74995824	-2.43385435	2.40260486
C	-0.42835961	3.82379465	1.39136172
C	3.55580105	1.00488392	1.10971218
C	2.93880487	2.22081208	0.91697777
H	3.22373397	-3.40169047	2.53975605
H	-0.92806367	4.77292747	1.22015545
H	1.46124956	4.48845066	0.63149532
H	3.48652613	3.05273366	0.48338440
H	4.59648766	0.86556265	0.83057083
H	4.49867503	-1.50528231	1.58208280
Ag	-0.68381145	-0.81821375	-2.91935827
Ag	-0.91993299	1.19758399	-4.79722339
Ag	-0.53605693	1.80353244	-2.10229118
Ag	-0.30413957	-0.26374387	-0.24980635
Ag	-0.46172065	-2.89984067	-1.13596596
Ag	-0.84699753	-3.41715724	-3.84910791
Ag	-1.09105031	-1.41294223	-5.78273929
Ag	-1.21959107	-4.05412996	-6.46033090

Ag -1.29539498 0.74210218 -7.44573435

g-Ag₉...Coronene

C	1.07154502	3.97168334	0.51739998
C	1.72800689	2.74861011	0.86783139
C	0.95155587	1.57410944	1.03680732
C	2.99851180	0.28351581	1.52883388
C	1.58928207	0.33510388	1.36983006
C	3.61670649	-0.97001614	1.84196450
C	1.44109029	-2.08615444	1.83059813
C	0.64258795	-3.26824197	1.95471689
C	0.80652294	-0.85499588	1.52688047
C	-0.72052371	-3.22434969	1.76761269
H	1.13574312	-4.20717288	2.18935497
C	-0.61172274	-0.80876080	1.33561311
C	-1.38030344	-1.99532237	1.44580041
H	-1.31670659	-4.12835591	1.85296153
C	-1.24748299	0.42762943	0.98911911
C	-2.79185830	-1.93357966	1.21183110
C	-2.64745884	0.46489199	0.75730550
C	-0.46637797	1.62008376	0.84420680
C	-3.40426509	-0.74558608	0.87861037
H	-3.37332108	-2.84722467	1.29654250
C	-3.25958916	1.70826330	0.39545434
C	-1.09363179	2.83899665	0.48235616
H	-4.47496195	-0.71014296	0.69785353
C	-2.50907615	2.85548311	0.26526633
H	-4.33166336	1.72842510	0.22074911
H	-2.98210406	3.79309073	-0.01231811
C	2.86449929	-2.11457164	1.98704127
C	-0.29176245	4.01538494	0.33049903

C	3.76171278	1.48361002	1.35936961
C	3.14756645	2.67436201	1.04117765
H	3.34333622	-3.06167232	2.21876554
H	-0.78018920	4.94599444	0.05613773
H	1.67274506	4.86781096	0.39268845
H	3.73534694	3.57859871	0.91092642
H	4.83998663	1.43666818	1.48379182
H	4.69622606	-1.00211152	1.96016339
Ag	0.88779572	-0.21561136	-3.39549558
Ag	-1.50582159	0.90932853	-4.09861612
Ag	0.81612201	2.42528398	-4.47921205
Ag	3.20765769	1.23723617	-3.75058234
Ag	3.29987324	-1.35391997	-2.68503965
Ag	1.00398811	-2.85354748	-2.30843576
Ag	-1.41464246	-1.65270492	-3.04504934
Ag	-1.26286026	-4.24397836	-1.97337154
Ag	-1.53875999	3.50850168	-5.16136873

h-Ag₉...Coronene

C	0.69306775	4.03715547	1.05277338
C	1.56319847	2.91309643	1.22311509
C	1.00672292	1.60904300	1.24881485
C	3.26322859	0.64417739	1.52261620
C	1.86038433	0.46838808	1.40014961
C	4.09929053	-0.51152140	1.65268754
C	2.14780487	-1.98025109	1.53548439
C	1.56899239	-3.28981027	1.51616487
C	1.29985131	-0.85046549	1.41207131
C	0.21165332	-3.46143581	1.36390443
H	2.22486981	-4.15020545	1.61308367
C	-0.11233903	-1.02891590	1.25710168

C	-0.66153152	-2.33581898	1.22278188
H	-0.21715801	-4.45916522	1.33935704
C	-0.96419693	0.11125931	1.09203022
C	-2.07161747	-2.49247891	1.02744573
C	-2.35861144	-0.06754829	0.89532112
C	-0.40517315	1.43056373	1.09248319
C	-2.89165158	-1.39716508	0.86857932
H	-2.48431995	-3.49696015	1.00068212
C	-3.18906030	1.08554740	0.71549615
C	-1.24633204	2.55713774	0.90968656
H	-3.95943005	-1.52669217	0.71563196
C	-2.65179292	2.35345262	0.72509343
H	-4.25532495	0.94008529	0.56652640
H	-3.28947551	3.22159066	0.58504409
C	3.56053965	-1.77903352	1.65823254
C	-0.66442278	3.86528344	0.90069270
C	3.80226921	1.97095894	1.50012386
C	2.98069691	3.06673182	1.35655196
H	4.20359275	-2.64953487	1.75145678
H	-1.31593001	4.72348217	0.76320772
H	1.12647334	5.03312492	1.03716531
H	3.39926992	4.06898037	1.33680904
H	4.87705135	2.09781883	1.59556421
H	5.17249617	-0.36915198	1.74392457
Ag	0.37235471	-0.28857391	-3.99617377
Ag	0.19679539	1.26979204	-1.75341953
Ag	0.02261930	2.53455010	-4.24429207
Ag	0.20649336	0.90929293	-6.47734631
Ag	0.54988804	-1.86395591	-6.25565724
Ag	0.72219994	-3.11524962	-3.79265615

Ag	0.53633057	-1.47228752	-1.53422210
Ag	0.88041083	-4.25463004	-1.37171642
Ag	-0.14699173	4.04265316	-2.03498792

i-Ag₉...Coronene

C	1.12923691	3.87189571	0.14311711
C	1.76990015	2.67258414	0.59128546
C	0.97395169	1.53950527	0.89702914
C	3.00714686	0.25230209	1.45108327
C	1.59498768	0.32312077	1.32999181
C	3.60771108	-0.97997694	1.86625654
C	1.40912167	-2.03780952	2.02872054
C	0.58953179	-3.18223031	2.29123887
C	0.79201367	-0.82647661	1.62558057
C	-0.77761447	-3.12292787	2.14156512
H	1.06946160	-4.10597802	2.60140953
C	-0.63030803	-0.76388161	1.47318460
C	-1.42054380	-1.91484185	1.72138585
H	-1.39024270	-3.99941218	2.33237289
C	-1.24986939	0.44854905	1.02701692
C	-2.83721546	-1.84111234	1.52479926
C	-2.65543325	0.49784272	0.83461419
C	-0.44810692	1.60170416	0.74332304
C	-3.43406560	-0.67613057	1.09585373
H	-3.43536454	-2.72761314	1.71547226
C	-3.25172445	1.71514961	0.37178295
C	-1.06004154	2.79504904	0.28332751
H	-4.50899672	-0.63185607	0.94457954
C	-2.48104029	2.82547720	0.10805859
H	-4.32816930	1.74483851	0.22805905
H	-2.94226722	3.74325651	-0.24530730

C	2.83587047	-2.08617159	2.14458314
C	-0.23810262	3.93103292	-0.00633001
C	3.79039553	1.41112723	1.14275586
C	3.19235017	2.58035024	0.72854403
H	3.30122169	-3.01797582	2.45307911
H	-0.71476520	4.84254181	-0.35534747
H	1.74544210	4.73660951	-0.08623058
H	3.79514399	3.45292885	0.49329633
H	4.87083732	1.34977535	1.23888282
H	4.68952013	-1.02718927	1.95470870
Ag	0.25241472	-0.92976681	-6.39230808
Ag	-0.19964254	-3.41068722	-5.01474998
Ag	2.45165099	-2.40509438	-5.47995301
Ag	-1.16615615	-3.28048578	-2.47442154
Ag	-0.75313756	-0.84959271	-3.83989115
Ag	1.44667030	-2.32530373	-2.92729895
Ag	-1.75373859	0.81875557	-5.75967721
Ag	4.04162307	-3.06898356	-3.35546639
Ag	0.82609626	-3.43991122	-7.53455506

j-Ag...Coronene

C	0.85390136	3.51274896	-2.69124231
C	1.42550766	2.44473761	-1.92817581
C	0.61364116	1.33519395	-1.58080491
C	2.53304801	0.27872062	-0.44172982
C	1.16934131	0.24669513	-0.83307415
C	3.07248222	-0.82958883	0.28780341
C	0.91041066	-1.96998082	0.22336445
C	0.08395581	-3.09931176	0.52655809
C	0.35294425	-0.88121554	-0.49391717
C	-1.22980706	-3.14487957	0.11795242

H	0.51769824	-3.92859264	1.07792823
C	-1.01450077	-0.92717985	-0.91596349
C	-1.80924217	-2.06366066	-0.62001857
H	-1.84600607	-4.01066043	0.34304793
C	-1.56611412	0.15529403	-1.67549163
C	-3.16290738	-2.10576772	-1.08569916
C	-2.90908870	0.09048287	-2.13076873
C	-0.75328373	1.28863484	-2.00399938
C	-3.69439348	-1.06578543	-1.81601844
H	-3.76463086	-2.98059410	-0.85628722
C	-3.43478517	1.17629615	-2.90295055
C	-1.29428376	2.35044235	-2.77212414
H	-4.72082423	-1.10957342	-2.16935051
C	-2.65523613	2.26905550	-3.21037902
H	-4.46379684	1.11933606	-3.24669760
H	-3.06216606	3.08628212	-3.79899204
C	2.28888503	-1.91589387	0.60840754
C	-0.46009070	3.46704550	-3.09963564
C	3.33232183	1.41243512	-0.79848293
C	2.79672156	2.45899815	-1.51552568
H	2.70884660	-2.75422457	1.15687319
H	-0.88284608	4.27794271	-3.68580324
H	1.48132065	4.36067643	-2.95086356
H	3.41192785	3.31290114	-1.78472117
H	4.37519846	1.43046801	-0.49444010
H	4.11783103	-0.79885215	0.58219217
Ag	0.60076486	-0.07438371	-5.20524211
Ag	1.23055193	-2.72483589	-6.11927694
Ag	2.52147781	-1.57426065	-3.82435316
Ag	-0.61189796	-4.67806786	-5.67810480

Ag	-1.24119870	-2.07065825	-4.81223618
Ag	0.68001345	-3.57092502	-3.43098833
Ag	-2.05837911	0.40595780	-5.63001124
Ag	3.00302624	-3.54647310	-1.99113396
Ag	3.03927039	-0.72085528	-6.45840968

k-Ag₉...Coronene

C	1.16688679	3.57395226	-1.41519653
C	1.73849309	2.50594091	-0.65213003
C	0.92662659	1.39639725	-0.30475913
C	2.84603344	0.33992392	0.83431596
C	1.48232674	0.30789843	0.44297163
C	3.38546765	-0.76838553	1.56384919
C	1.22339609	-1.90877752	1.49941023
C	0.39694124	-3.03810846	1.80260387
C	0.66592968	-0.82001224	0.78212861
C	-0.91682163	-3.08367627	1.39399820
H	0.83068367	-3.86738934	2.35397401
C	-0.70151534	-0.86597655	0.36008229
C	-1.49625674	-2.00245736	0.65602721
H	-1.53302064	-3.94945713	1.61909371
C	-1.25312869	0.21649733	-0.39944585
C	-2.84992195	-2.04456442	0.19034662
C	-2.59610327	0.15168617	-0.85472295
C	-0.44029830	1.34983814	-0.72795360
C	-3.38140805	-1.00458213	-0.53997266
H	-3.45164543	-2.91939080	0.41975856
C	-3.12179974	1.23749945	-1.62690477
C	-0.98129833	2.41164565	-1.49607836
H	-4.40783880	-1.04837012	-0.89330473
C	-2.34225070	2.33025880	-1.93433324

H	-4.15081141	1.18053936	-1.97065182
H	-2.74918063	3.14748542	-2.52294626
C	2.60187046	-1.85469057	1.88445332
C	-0.14710527	3.52824880	-1.82358986
C	3.64530726	1.47363842	0.47756285
C	3.10970699	2.52020145	-0.23947990
H	3.02183203	-2.69302127	2.43291897
H	-0.56986065	4.33914601	-2.40975746
H	1.79430608	4.42187973	-1.67481778
H	3.72491328	3.37410444	-0.50867539
H	4.68818389	1.49167131	0.78160568
H	4.43081646	-0.73764885	1.85823795
Ag	-0.14081256	-2.80032044	-5.18559596
Ag	1.19079510	-1.38554258	-3.06847225
Ag	2.01042852	-4.02029530	-3.87051172
Ag	2.79742753	0.69747972	-3.76425954
Ag	1.46398214	-0.67108686	-5.83628311
Ag	3.61578234	-1.89137879	-4.52085708
Ag	-0.94169254	-1.00684887	-7.08934342
Ag	4.72719366	-4.22169012	-3.62387274
Ag	-0.38462214	-3.52257209	-2.47384871

a-Ag₁₀...Coronene

C	1.01203200	3.93177000	0.25719900
C	1.69674100	2.69701300	0.49426700
C	0.94369500	1.54900500	0.84906300
C	3.01594300	0.20903800	0.93865800
C	1.60608000	0.29853900	1.07337200
C	3.65474500	-1.05575600	1.14790900
C	1.49741800	-2.10819100	1.61430000
C	0.71331600	-3.26399300	1.92997100

C	0.84400900	-0.86510200	1.41819300
C	-0.65746400	-3.18405800	2.02785100
H	1.22126200	-4.21223300	2.08057000
C	-0.58149500	-0.78130200	1.52334800
C	-1.33933500	-1.94271000	1.81931400
H	-1.24493900	-4.06856500	2.25690600
C	-1.24481600	0.46623700	1.28552100
C	-2.76677400	-1.84441800	1.88093800
C	-2.66108400	0.53976800	1.34746100
C	-0.48178700	1.63251000	0.95285600
C	-3.40568900	-0.64567300	1.65245400
H	-3.34022200	-2.73899800	2.10656200
C	-3.30431100	1.79330500	1.08955400
C	-1.14040300	2.86204300	0.69868000
H	-4.48939500	-0.58256200	1.69626400
C	-2.56925300	2.91554000	0.77873200
H	-4.38848300	1.84129900	1.13994400
H	-3.06645700	3.86105600	0.58199800
C	2.92118400	-2.17499600	1.47357800
C	-0.35890200	4.01152400	0.35532300
C	3.75655700	1.38300000	0.58549500
C	3.11912600	2.58483800	0.37200200
H	3.41432300	-3.13104000	1.62449000
H	-0.87066800	4.95055500	0.16509900
H	1.59605500	4.80750900	-0.01119900
H	3.68907500	3.46896600	0.10076200
H	4.83570500	1.30710600	0.48530200
H	4.73418400	-1.11696700	1.04100600
Ag	-1.16294307	-1.54822133	-4.85442116
Ag	-2.25784107	2.47401567	-2.55150916

Ag	-0.71725107	3.01347767	-4.85442116
Ag	-2.25784107	-0.80829233	-7.25526716
Ag	-2.64973407	0.77478567	-4.85442116
Ag	-0.11809007	0.72327267	-6.29268316
Ag	-2.25784107	2.47401567	-7.15733316
Ag	-2.25784107	-0.80829233	-2.45357516
Ag	-3.54528707	3.37429167	-4.85442116
Ag	-0.11809007	0.72327267	-3.41615916

b-Ag₁₀...Coronene

C	1.02498817	3.85210110	0.06198550
C	1.70969717	2.61734410	0.29905350
C	0.95665117	1.46933610	0.65384950
C	3.02889917	0.12936910	0.74344450
C	1.61903617	0.21887010	0.87815850
C	3.66770117	-1.13542490	0.95269550
C	1.51037417	-2.18785990	1.41908650
C	0.72627217	-3.34366190	1.73475750
C	0.85696517	-0.94477090	1.22297950
C	-0.64450783	-3.26372690	1.83263750
H	1.23421817	-4.29190190	1.88535650
C	-0.56853883	-0.86097090	1.32813450
C	-1.32637883	-2.02237890	1.62410050
H	-1.23198283	-4.14823390	2.06169250
C	-1.23185983	0.38656810	1.09030750
C	-2.75381783	-1.92408690	1.68572450
C	-2.64812783	0.46009910	1.15224750
C	-0.46883083	1.55284110	0.75764250
C	-3.39273283	-0.72534190	1.45724050
H	-3.32726583	-2.81866690	1.91134850
C	-3.29135483	1.71363610	0.89434050

C	-1.12744683	2.78237410	0.50346650
H	-4.47643883	-0.66223090	1.50105050
C	-2.55629683	2.83587110	0.58351850
H	-4.37552683	1.76163010	0.94473050
H	-3.05350083	3.78138710	0.38678450
C	2.93414017	-2.25466490	1.27836450
C	-0.34594583	3.93185510	0.16010950
C	3.76951317	1.30333110	0.39028150
C	3.13208217	2.50516910	0.17678850
H	3.42727917	-3.21070890	1.42927650
H	-0.85771183	4.87088610	-0.03011450
H	1.60901117	4.72784010	-0.20641250
H	3.70203117	3.38929710	-0.09445150
H	4.84866117	1.22743710	0.29008850
H	4.74714017	-1.19663590	0.84579250
Ag	2.54013207	0.57533516	-3.29781924
Ag	-2.04933623	1.83787740	-3.45067060
Ag	-1.66519990	-0.72043780	-4.57996378
Ag	2.14798402	-1.75443934	-1.90903244
Ag	0.00207841	0.15993506	-2.30150836
Ag	0.97199447	-1.55679640	-4.44453623
Ag	-0.97495035	-2.54779652	-2.54227977
Ag	1.02790863	2.81774045	-2.85605365
Ag	-2.66032548	-0.41449044	-1.92589226
Ag	0.30099688	1.18223495	-5.01186317

CORDINATES FOR (dodecabenzocoronene) DBC

C	2.64342	1.08318	0.00012
C	-2.64342	-1.08318	-0.00010
C	2.25999	-1.74737	-0.00013
C	-2.25999	1.74736	0.00009
C	3.76553	0.2125	0.00000

C	3.5734	-1.20651	0.00001
C	0.74166	-3.69749	0.00000
C	-0.38344	-2.83056	0.00011
C	-1.69869	-3.36685	0.00000
C	-2.83164	-2.49082	-0.00001
C	-3.76552	-0.2125	0.00000
C	-3.5734	1.20651	0.00001
C	-2.06704	3.15437	0.00001
C	-0.74166	3.69749	0.00000
C	0.38344	2.83056	-0.00010
C	1.69869	3.36685	-0.00001
C	2.83164	2.49082	0.00000
C	0.19066	1.40744	0.00026
C	-0.19065	-1.40744	-0.00028
C	-1.31428	-0.53853	0.00025
C	-1.12371	0.86887	-0.00024
C	1.12371	-0.86887	0.00030
C	1.31428	0.53853	-0.00029
C	2.06704	-3.15437	0.00001
C	0.5446	-5.1127	0.00006
C	3.20079	-4.02424	-0.00005
C	4.49357	-3.47408	-0.00009
C	4.70076	-2.08456	-0.00005
H	5.35407	-4.13903	-0.00012
C	-0.76253	-5.62788	0.00009
C	-1.88548	-4.78338	0.00005
H	-0.90894	-6.70548	0.00011
C	4.15593	3.02779	0.00005
C	5.25566	2.1536	0.00009
H	6.2619	2.56604	0.00011
C	5.08582	0.75917	0.00006
C	-4.15593	-3.02779	-0.00007
C	-5.25566	-2.1536	-0.00010
H	-6.2619	-2.56604	-0.00013
C	-5.08583	-0.75917	-0.00006
C	1.88548	4.78339	-0.00006
C	0.76253	5.62788	-0.00009
H	0.90893	6.70548	-0.00011
C	-0.5446	5.11269	-0.00006
C	-3.20079	4.02424	0.00006
C	-4.49357	3.47408	0.00010
H	-5.35407	4.13903	0.00012
C	-4.70076	2.08457	0.00006
C	-3.23677	-5.30136	0.00002
C	-4.31763	-4.46544	-0.00004
C	3.23677	5.30136	-0.00004
C	4.31763	4.46544	0.00002
H	5.32634	4.86811	0.00004
C	-2.97375	5.45322	0.00004
C	-1.70925	5.97136	-0.00003
C	-6.21009	0.15149	-0.00003
C	-6.02685	1.50554	0.00004

C	6.21009	-0.15149	0.00003
C	6.02685	-1.50554	-0.00002
C	1.70925	-5.97136	0.00004
C	2.97375	-5.45322	-0.00002
H	3.37355	6.37888	-0.00006
H	-1.55358	7.04628	-0.00005
H	-3.83896	6.10978	0.00006
H	-6.88039	2.17724	0.00006
H	-7.21131	-0.26949	-0.00005
H	-5.32634	-4.86811	-0.00007
H	-3.37355	-6.37888	0.00004
H	1.55358	-7.04628	0.00007
H	3.83896	-6.10979	-0.00004
H	6.88038	-2.17724	-0.00005
H	7.21131	0.26949	0.00006