

The role of covalency in enhancing stability of Eu and Am complexes: A DFT comparison of BTP and
BTPhen

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1. BHLYP-optimised and B3LYP-optimised Cartesian coordinates of all structures, obtained using the def(2)-SVP basis set and the COSMO continuum solvent model.

Eu(H₂O)₉

BHLYP

Eu	0.0097529	-0.0000378	-0.0047579
O	0.0038761	1.6487746	1.7879017
O	2.1489085	-0.0003933	1.2208750
O	0.0147020	-0.0001083	-2.4711240
O	-1.5376702	-1.6583733	-0.8902834
O	1.5403763	-1.6635036	-0.8898933
O	0.0051824	-1.6487527	1.7875453
O	-2.1416886	-0.0001885	1.2258835
O	-1.5370309	1.6583417	-0.8916690
O	1.5413057	1.6634367	-0.8881132
H	1.3964769	-2.1634615	-1.6955012
H	2.1677201	-2.1705637	-0.3711095
H	-2.1933542	-2.1342650	-0.3772952
H	-1.4243125	-2.1553137	-1.7026012
H	-0.7596006	-2.1424189	2.0891309
H	0.7725485	-2.1339969	2.0963983
H	-3.0209731	0.0005440	0.8419227
H	-2.2695332	0.0002837	2.1768277
H	2.2707379	0.0002079	2.1726214
H	3.0301572	-0.0004833	0.8411919
H	-0.7544507	0.0000212	-3.0447979
H	0.7783961	0.0005718	-3.0520838
H	1.4005621	2.1661257	-1.6926048
H	2.1677762	2.1681153	-0.3659669
H	-2.1945737	2.1358139	-0.3825227
H	-1.4214078	2.1525165	-1.7053384
H	-0.7629822	2.1408127	2.0868274
H	0.7690986	2.1362949	2.0985367

B3LYP

Eu	0.0156966	-0.0001037	-0.0066145
O	0.0037168	1.6478913	1.8026633
O	2.1604508	-0.0008913	1.2171406
O	0.0265515	0.0011971	-2.4798308
O	-1.5504114	-1.6544842	-0.8991547
O	1.5506396	-1.6699784	-0.8960938
O	0.0059830	-1.6489925	1.8017107
O	-2.1466560	-0.0003914	1.2322636
O	-1.5494969	1.6553139	-0.8997949
O	1.5518097	1.6698781	-0.8938205
H	1.3786340	-2.1868546	-1.6984063
H	2.1479258	-2.2128292	-0.3583818

H	-2.1880476	-2.1488482	-0.3612912
H	-1.4051259	-2.1935423	-1.6920699
H	-0.7731926	-2.1541976	2.0807653
H	0.7713065	-2.1756797	2.0797711
H	-3.0370979	0.0023538	0.8475114
H	-2.2781195	-0.0025601	2.1934086
H	2.2863392	0.0031051	2.1789175
H	3.0514627	-0.0016019	0.8336517
H	-0.7502670	-0.0027980	-3.0608334
H	0.7968009	0.0024509	-3.0695772
H	1.3832909	2.1911203	-1.6940417
H	2.1515065	2.2070491	-0.3531235
H	-2.1852620	2.1564606	-0.3660022
H	-1.4024758	2.1872014	-1.6972156
H	-0.7800917	2.1472975	2.0791852
H	0.7641299	2.1824341	2.0792630

Am(H₂O)₉

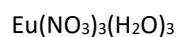
BHLYP

Am	0.0050769	-0.0000248	-0.0011115
O	0.0012094	1.6614900	1.8511282
O	2.1654720	-0.0002968	1.2425187
O	0.0043694	-0.0001132	-2.4943286
O	-1.5939436	-1.6694470	-0.9214735
O	1.6029775	-1.6676871	-0.9270055
O	0.0027777	-1.6617150	1.8504535
O	-2.1629958	-0.0004273	1.2406571
O	-1.5933265	1.6695278	-0.9227378
O	1.6041999	1.6675767	-0.9254977
H	1.4746321	-2.1580874	-1.7413313
H	2.2452659	-2.1663980	-0.4180868
H	-2.2556316	-2.1414124	-0.4120770
H	-1.4877534	-2.1633489	-1.7369214
H	-0.7638524	-2.1484525	2.1594554
H	0.7674709	-2.1447758	2.1699689
H	-3.0437043	0.0004573	0.8595178
H	-2.2889476	-0.0001036	2.1920481
H	2.2865308	0.0005019	2.1944806
H	3.0477718	-0.0004671	0.8649314
H	-0.7647462	-0.0000181	-3.0682650
H	0.7674337	0.0009248	-3.0763601
H	1.4792603	2.1607076	-1.7387338
H	2.2460296	2.1635707	-0.4133769
H	-2.2566915	2.1431805	-0.4170803
H	-1.4848961	2.1606627	-1.7395560
H	-0.7675963	2.1467767	2.1569412
H	0.7636074	2.1473979	2.1718426

B3LYP

Am	0.0224576	-0.0000867	-0.0102202
O	0.0065111	1.6736373	1.8431946
O	2.2091787	-0.0009538	1.2116016
O	0.0536441	0.0006925	-2.5163959
O	-1.5827027	-1.6819082	-0.9215704
O	1.5669558	-1.7176510	-0.9064702
O	0.0081790	-1.6741516	1.8422834
O	-2.1862714	-0.0006886	1.2538457
O	-1.5819413	1.6822043	-0.9225460
O	1.5680616	1.7176672	-0.9038565
H	1.4143185	-2.2274532	-1.7174167
H	2.1897816	-2.2430946	-0.3801384
H	-2.2532734	-2.1511237	-0.4010342
H	-1.4666847	-2.2072891	-1.7287880
H	-0.7737459	-2.1559430	2.1542680
H	0.7700866	-2.1902980	2.1492017
H	-3.0790246	0.0009071	0.8743097
H	-2.3181874	-0.0005652	2.2149355
H	2.3437936	0.0015428	2.1723721
H	3.0990878	-0.0011598	0.8249980

H	-0.7173902	-0.0008388	-3.1053048
H	0.8272294	0.0012248	-3.1020622
H	1.4194324	2.2305758	-1.7136488
H	2.1914078	2.2392724	-0.3743210
H	-2.2538861	2.1541581	-0.4062552
H	-1.4639966	2.2034147	-1.7321626
H	-0.7782666	2.1532651	2.1513364
H	0.7652453	2.1946430	2.1498445

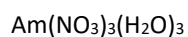


BHLYP

Eu	0.0833337	-0.3095752	0.0762213
N	2.9788606	-0.1009617	0.1845115
N	-0.0072285	2.5619413	-0.1081704
N	-2.8091558	-0.3040370	0.1263374
O	2.2469039	0.4611429	1.0281661
O	2.3822990	-0.7735759	-0.6863518
O	-2.1520554	-0.0072934	-0.8982950
O	-2.1342972	-0.6070769	1.1322553
O	-0.4326731	1.9402423	0.8917661
O	0.4445746	1.8561743	-1.0360791
O	-4.0001346	-0.2970644	0.1369825
O	-0.0342783	3.7513149	-0.1712786
O	4.1653942	-0.0040644	0.2074010
O	-0.1605841	-2.6952840	-0.0814830
H	-0.2177654	-3.1344459	-0.9326880
O	0.3359806	-1.0683201	2.3384985
H	1.1059041	-0.8611731	2.8726549
H	-0.3673575	-1.3118881	2.9438887
O	0.1083546	-0.9699427	-2.2589322
H	0.9042779	-0.9799041	-2.7946463
H	-0.6270748	-0.8267430	-2.8583246
H	-0.4247629	-3.3333623	0.5837405

B3LYP

Eu	0.0735393	-0.3219590	0.0921784
N	2.9770136	-0.0552168	0.2144327
N	0.0098414	2.5586381	-0.1547612
N	-2.8287440	-0.2952254	0.1617369
O	2.2153974	0.5104668	1.0624806
O	2.3911810	-0.7843161	-0.6500277
O	-2.1703855	-0.0633474	-0.9044744
O	-2.1315746	-0.5664000	1.1897405
O	-0.4492776	1.9467082	0.8646631
O	0.4608506	1.8199332	-1.0863668
O	-4.0373854	-0.2576796	0.1918844
O	0.0136460	3.7665575	-0.2294054
O	4.1773665	0.0909465	0.2268389
O	-0.1660721	-2.7229376	-0.0994913
H	-0.2997189	-3.0971921	-0.9848370
O	0.3805298	-1.1408672	2.3447668
H	1.1202935	-0.8325577	2.8918550
H	-0.3241491	-1.3996826	2.9592120
O	0.1145317	-1.0185495	-2.2658649
H	0.9400180	-0.9949104	-2.7755337
H	-0.5898023	-0.7744182	-2.8869339
H	-0.4885835	-3.3818871	0.5340818

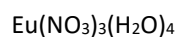


BHLYP

Am	-0.0389513	-0.2763920	0.0107357
N	2.8974431	-0.2798011	0.0763189
N	0.1456229	2.6618570	-0.0192681
N	-2.9642697	-0.0065146	0.0685300
O	2.2129343	0.1705071	1.0227159
O	2.2474775	-0.7687913	-0.8757816
O	-2.2928301	0.2104283	-0.9668575
O	-2.3081817	-0.3488466	1.0764630
O	-0.3408461	2.0247815	0.9434615
O	0.5410171	1.9744984	-0.9855450
O	-4.1491067	0.1044586	0.0888182
O	0.2227190	3.8512500	-0.0132643
O	4.0866859	-0.2461536	0.0810954
O	-0.5034044	-2.6723861	-0.3032285
H	-0.6027843	-3.0530926	-1.1786084
O	0.0800390	-1.2062021	2.2695828
H	0.8737648	-1.1890419	2.8089917
H	-0.6581877	-1.3507749	2.8653064
O	-0.0823750	-0.8091093	-2.4077911
H	0.7018606	-0.8227163	-2.9604777
H	-0.8204427	-0.6019542	-2.9849860
H	-0.8098165	-3.3310416	0.3230435

B3LYP

Am	0.0768997	-0.3048614	0.0949825
N	3.0154570	-0.0609295	0.2093276
N	0.0255023	2.6316202	-0.1640478
N	-2.8712687	-0.2743176	0.1614238
O	2.2599574	0.4242149	1.1137685
O	2.4177624	-0.6847071	-0.7273457
O	-2.2190822	-0.0847359	-0.9169344
O	-2.1647327	-0.4750730	1.2018551
O	-0.4003371	2.0189929	0.8711613
O	0.4579998	1.8922565	-1.1045318
O	-4.0794873	-0.2657321	0.1942688
O	0.0158735	3.8389576	-0.2428779
O	4.2170738	0.0626753	0.2376277
O	-0.1465491	-2.7538616	-0.1004576
H	-0.2219603	-3.1903962	-0.9636356
O	0.3005465	-1.1823544	2.3863125
H	1.0804505	-0.9993432	2.9341228
H	-0.4305393	-1.3513535	3.0014445
O	0.0933367	-1.0174207	-2.3060856
H	0.8937877	-0.9673519	-2.8521798
H	-0.6475881	-0.8322366	-2.9046453
H	-0.2845869	-3.4379391	0.5726212



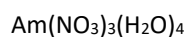
BHLYP

Eu	0.8412857	0.0545926	-0.0699300
N	3.6970385	-0.6074277	-0.1928298
N	-0.0762729	2.7659343	0.5806617
N	-1.1239326	-2.0278299	-0.6033572
O	3.2236932	0.3066661	0.5177056
O	2.8950833	-1.1903079	-0.9460783
O	-1.2865023	-1.1878556	0.3056889
O	-0.0707975	-1.9293304	-1.2665509
O	-0.7571274	1.7851251	0.9321119
O	1.0246365	2.5110823	0.0436428
O	-1.9326382	-2.8801885	-0.8268385
O	-0.4482059	3.8907325	0.7447426
O	4.8555427	-0.9009031	-0.1478153
O	1.4237980	-2.0047847	1.1971124
H	1.0382704	-2.1762715	2.0577080
O	1.7160904	0.8881298	-2.2081950
H	2.4691837	0.4802957	-2.6389931
O	1.0133749	0.3434182	2.3631857
H	0.4580279	0.9621510	2.8402416
H	1.8584163	0.3197957	2.8164939
O	-0.8800876	0.8930536	-1.6467909
H	-0.7677532	0.7941276	-2.5934511
H	-1.8223716	0.8827560	-1.4741177
H	1.7670071	1.8288995	-2.3891978
H	1.5555985	-2.8560264	0.7774533

B3LYP

Eu	0.8432219	0.0597053	-0.0653732
N	3.7222138	-0.5485526	-0.1756479
N	-0.0116043	2.8077770	0.5800617
N	-1.1303450	-2.0405510	-0.5960529
O	3.2130468	0.3548227	0.5626348
O	2.9238146	-1.1401031	-0.9631603
O	-1.3003611	-1.1801718	0.3239425
O	-0.0568953	-1.9384569	-1.2697401
O	-0.7114963	1.8295799	0.9772978
O	1.0891460	2.5139601	0.0102884
O	-1.9466220	-2.9112771	-0.8192946
O	-0.3627603	3.9597123	0.7309716
O	4.9034242	-0.8225504	-0.1261260
O	1.4656030	-2.0376578	1.1836492
H	1.0021419	-2.2068370	2.0183944
O	1.6534153	0.8669899	-2.2755243
H	2.4450337	0.4334042	-2.6315822
O	0.9608588	0.2642495	2.4082011
H	0.4138236	0.9598817	2.8058219
H	1.8265277	0.3210374	2.8428920
O	-0.9203669	0.9242992	-1.6243319
H	-0.7673515	0.7811778	-2.5711091

H	-1.8636325	0.7606545	-1.4747666
H	1.7937878	1.8201422	-2.3930485
H	1.4867338	-2.8854017	0.7142048



BHLYP

Am	0.8480930	0.0587337	-0.0607276
N	3.7329804	-0.6033127	-0.1879149
N	-0.0751812	2.8016198	0.5780364
N	-1.1538015	-2.0604699	-0.6110139
O	3.2810926	0.3096927	0.5363170
O	2.9095091	-1.1708173	-0.9347636
O	-1.3159920	-1.2223131	0.3007697
O	-0.0995839	-1.9632613	-1.2730739
O	-0.7348220	1.8058772	0.9387229
O	1.0267861	2.5658216	0.0366605
O	-1.9645218	-2.9101860	-0.8371038
O	-0.4718071	3.9170836	0.7389322
O	4.8864202	-0.9137764	-0.1655214
O	1.4421222	-2.0490827	1.2231212
H	1.0386882	-2.2297411	2.0738946
O	1.7260965	0.9054417	-2.2506956
H	2.4781794	0.4937480	-2.6802027
O	1.0155386	0.3450583	2.4183693
H	0.4610409	0.9761971	2.8807910
H	1.8550210	0.3253035	2.8824255
O	-0.9147885	0.9117335	-1.6711189
H	-0.7923318	0.8160308	-2.6170737
H	-1.8593384	0.8882309	-1.5114161
H	1.7895993	1.8460980	-2.4290790
H	1.5623585	-2.8978754	0.7942676

B3LYP

Am	0.8512404	0.0673970	-0.0603770
N	3.7537291	-0.5614229	-0.1729416
N	-0.0364726	2.8294246	0.5848241
N	-1.1598733	-2.0635799	-0.6154118
O	3.2752453	0.3609245	0.5617917
O	2.9266539	-1.1444927	-0.9419812
O	-1.3230467	-1.2140007	0.3164293
O	-0.0904266	-1.9558536	-1.2947971
O	-0.7112609	1.8215244	0.9631454
O	1.0747825	2.5743583	0.0189271
O	-1.9799381	-2.9298273	-0.8440615
O	-0.4266076	3.9655262	0.7500005
O	4.9271071	-0.8652147	-0.1399670
O	1.4634616	-2.0678091	1.2148930
H	1.0148653	-2.2447977	2.0562194
O	1.6834592	0.8781467	-2.3049030
H	2.4702061	0.4476790	-2.6752426
O	0.9828902	0.2880966	2.4503159
H	0.4338938	0.9684340	2.8710190
H	1.8434929	0.3265994	2.8971483
O	-0.9401022	0.9426712	-1.6630399
H	-0.8105536	0.7807111	-2.6103521

H	-1.8899420	0.8365360	-1.5016645
H	1.8066022	1.8293345	-2.4537661
H	1.5319520	-2.9245305	0.7663945

EuBTP₃

BHLYP

Eu	0.0001523	-0.0046511	-0.0000817
N	-1.2792103	2.2362179	-0.0053527
C	-2.2444383	2.4648346	0.8815271
C	-0.9810466	3.1840204	-0.8901170
C	-2.9553154	3.6579041	0.9197666
C	-2.5462897	1.3885936	1.8503117
C	-1.6367397	4.4083666	-0.9220824
C	0.0918087	2.8894692	-1.8644806
C	-2.6411479	4.6444346	0.0009076
H	-3.7323439	3.7954270	1.6583806
N	-3.4740520	1.6136746	2.7750164
N	-1.8740793	0.2555428	1.7411090
H	-1.3564017	5.1476792	-1.6589656
N	0.7113471	1.7255439	-1.7663356
N	0.3774946	3.8058198	-2.7841134
H	-3.1739844	5.5876394	0.0037179
C	-3.7049386	0.6447142	3.6203628
N	-2.0977140	-0.7229083	2.5858357
N	1.6579257	1.4144093	-2.6199702
C	1.3206473	3.5062241	-3.6367090
C	-2.9917271	-0.5597070	3.5250308
H	-4.4547042	0.7917646	4.3918991
C	1.9777160	2.2691151	-3.5552500
H	1.5818978	4.2297065	-4.4030814
H	-3.1555799	-1.3810312	4.2125112
H	2.7595890	1.9862735	-4.2500049
N	-1.2969134	-2.2454978	0.0009524
C	-2.2685221	-2.4648572	-0.8805901
C	-1.0045244	-3.1949356	0.8853408
C	-2.9940192	-3.6492941	-0.9129567
C	-2.5614023	-1.3863884	-1.8494208
C	-1.6742540	-4.4116851	0.9232784
C	0.0784526	-2.9114842	1.8520445
C	-2.6867400	-4.6374540	0.0066204
H	-3.7765372	-3.7791671	-1.6471555
N	-3.5037142	-1.5973477	-2.7631419
N	-1.8679758	-0.2649847	-1.7513551
H	-1.3981387	-5.1530700	1.6596944
N	0.7093555	-1.7542031	1.7485864
N	0.3620161	-3.8305469	2.7696584
H	-3.2309596	-5.5741339	0.0088849
C	-3.7284751	-0.6265273	-3.6076732
N	-2.0841664	0.7147562	-2.5973015
N	1.6690018	-1.4537519	2.5915000
C	1.3170167	-3.5411165	3.6126762
C	-2.9922302	0.5651698	-3.5248929
H	-4.4909867	-0.7616651	-4.3688388
C	1.9889332	-2.3126437	3.5229232
H	1.5765100	-4.2665321	4.3778262
H	-3.1495386	1.3872511	-4.2130056
H	2.7822629	-2.0396624	4.2085907

N	2.5797003	0.0101800	0.0035760
C	3.2506185	0.7433654	0.8880574
C	3.2608475	-0.7081399	-0.8855307
C	4.6386713	0.7926662	0.9170928
C	2.4578399	1.5210672	1.8647570
C	4.6494470	-0.7221042	-0.9269085
C	2.4798883	-1.5092423	-1.8531729
C	5.3459238	0.0447764	-0.0086302
H	5.1381589	1.4059939	1.6536750
N	3.1071729	2.2243949	2.7869977
N	1.1401671	1.4745414	1.7654320
H	5.1576900	-1.3233681	-1.6674470
N	1.1626748	-1.4951380	-1.7423734
N	3.1384062	-2.1996077	-2.7786202
H	6.4291187	0.0590128	-0.0140526
C	2.3746141	2.8877541	3.6412216
N	0.3960877	2.1368303	2.6191842
N	0.4267709	-2.1783227	-2.5868089
C	2.4145144	-2.8850339	-3.6229289
C	0.9749253	2.8387137	3.5571451
H	2.8692092	3.4728465	4.4106845
C	1.0147545	-2.8703503	-3.5265949
H	2.9164182	-3.4606085	-4.3948233
H	0.3379979	3.3730070	4.2520624
H	0.3850662	-3.4225401	-4.2140707

B3LYP

Eu	0.0020490	-0.0031914	0.0016454
N	-1.2802948	2.2424822	-0.0058124
C	-2.2542320	2.4766076	0.8906563
C	-0.9851207	3.1980934	-0.9032938
C	-2.9711793	3.6799124	0.9242384
C	-2.5577928	1.4010280	1.8682856
C	-1.6499702	4.4309670	-0.9352428
C	0.0886615	2.9041520	-1.8851606
C	-2.6590698	4.6712965	-0.0043601
H	-3.7528160	3.8181324	1.6705307
N	-3.4925233	1.6325105	2.8002263
N	-1.8780135	0.2513780	1.7587595
H	-1.3689961	5.1731614	-1.6816367
N	0.7208729	1.7262165	-1.7835846
N	0.3706882	3.8273810	-2.8146587
H	-3.1971684	5.6212723	-0.0029571
C	-3.7228896	0.6557324	3.6589107
N	-2.1012176	-0.7318612	2.6194264
N	1.6749153	1.4144334	-2.6490657
C	1.3222538	3.5239028	-3.6785916
C	-3.0045201	-0.5540916	3.5701800
H	-4.4794220	0.8086820	4.4355678
C	1.9868845	2.2833141	-3.5971469
H	1.5793519	4.2541492	-4.4528754
H	-3.1651486	-1.3780400	4.2695445

H	2.7735435	1.9980771	-4.2996712
N	-1.3009836	-2.2531281	0.0013865
C	-2.2814532	-2.4771053	-0.8894235
C	-1.0091170	-3.2128603	0.8950864
C	-3.0123450	-3.6722392	-0.9194166
C	-2.5762529	-1.3973360	-1.8648407
C	-1.6869202	-4.4387595	0.9309933
C	0.0766663	-2.9317494	1.8679260
C	-2.7054881	-4.6670755	0.0073484
H	-3.8000589	-3.8018086	-1.6608554
N	-3.5226342	-1.6147257	-2.7887817
N	-1.8777411	-0.2578647	-1.7619668
H	-1.4088489	-5.1847440	1.6747123
N	0.7206338	-1.7609591	1.7607998
N	0.3573617	-3.8585544	2.7946405
H	-3.2546377	-5.6106995	0.0098045
C	-3.7472970	-0.6344844	-3.6448365
N	-2.0959480	0.7288459	-2.6204739
N	1.6867964	-1.4588785	2.6172242
C	1.3208796	-3.5653019	3.6489473
C	-3.0109661	0.5649247	-3.5622233
H	-4.5135904	-0.7760019	-4.4140680
C	1.9982552	-2.3319069	3.5616163
H	1.5777333	-4.2983515	4.4206754
H	-3.1672059	1.3919808	-4.2589212
H	2.7944850	-2.0555946	4.2569105
N	2.5868537	0.0137371	0.0034931
C	3.2664872	0.7478217	0.9008208
C	3.2765654	-0.7087706	-0.8959950
C	4.6664161	0.7932332	0.9296831
C	2.4734956	1.5262514	1.8848586
C	4.6771223	-0.7228120	-0.9331378
C	2.4963016	-1.5109283	-1.8720913
C	5.3792426	0.0438767	-0.0047595
H	5.1684496	1.4076208	1.6763252
N	3.1297275	2.2305336	2.8171244
N	1.1374053	1.4828138	1.7818489
H	5.1879600	-1.3276308	-1.6816211
N	1.1611095	-1.4996463	-1.7588494
N	3.1631495	-2.2032346	-2.8058185
H	6.4709417	0.0564237	-0.0087935
C	2.3889474	2.8993500	3.6819294
N	0.3882272	2.1499250	2.6479449
N	0.4202346	-2.1858663	-2.6175761
C	2.4313885	-2.8926760	-3.6624348
C	0.9823168	2.8531129	3.5984125
H	2.8907953	3.4854318	4.4588113
C	1.0246708	-2.8781814	-3.5698458
H	2.9410760	-3.4704421	-4.4404414
H	0.3403493	3.3891756	4.3014831
H	0.3905977	-3.4304393	-4.2675487

AmBTP₃

BHLYP

Am	0.0003736	-0.0000951	0.0000630
N	-1.3071474	2.2631317	-0.0010859
C	-2.2843535	2.4810040	0.8763070
C	-1.0076213	3.2178060	-0.8791789
C	-3.0067195	3.6673812	0.9097721
C	-2.5880825	1.4030737	1.8434950
C	-1.6755714	4.4356054	-0.9145689
C	0.0791585	2.9425189	-1.8449869
C	-2.6929218	4.6592859	-0.0031355
H	-3.7925877	3.7954957	1.6406009
N	-3.5193241	1.6262619	2.7659506
N	-1.9128923	0.2718703	1.7384370
H	-1.3936827	5.1799574	-1.6456948
N	0.7220379	1.7927576	-1.7388468
N	0.3516743	3.8604776	-2.7675259
H	-3.2354761	5.5969230	-0.0042390
C	-3.7485985	0.6579299	3.6121315
N	-2.1313810	-0.7054372	2.5867502
N	1.6790466	1.4939507	-2.5857786
C	1.3061618	3.5754377	-3.6124912
C	-3.0278085	-0.5430931	3.5238193
H	-4.5022739	0.8025626	4.3802786
C	1.9870893	2.3514849	-3.5227022
H	1.5577844	4.3002776	-4.3807770
H	-3.1881758	-1.3620705	4.2148432
H	2.7777682	2.0814387	-4.2125118
N	-1.3072089	-2.2632885	0.0011248
C	-2.2844535	-2.4811352	-0.8762370
C	-1.0081512	-3.2177024	0.8796533
C	-3.0072315	-3.6672703	-0.9093248
C	-2.5879228	-1.4033519	-1.8436734
C	-1.6765011	-4.4352740	0.9154135
C	0.0788186	-2.9425351	1.8452829
C	-2.6935350	-4.6591273	0.0036741
H	-3.7933571	-3.7952284	-1.6399037
N	-3.5189207	-1.6266896	-2.7663499
N	-1.9129142	-0.2720538	-1.7384542
H	-1.3951403	-5.1793285	1.6470455
N	0.7223271	-1.7931746	1.7385438
N	0.3513086	-3.8604650	2.7678549
H	-3.2359317	-5.5968541	0.0045930
C	-3.7481520	-0.6583968	-3.6125802
N	-2.1312634	0.7051722	-2.5869039
N	1.6792752	-1.4943154	2.5855336
C	1.3062257	-3.5756878	3.6124262
C	-3.0274511	0.5426748	-3.5241658
H	-4.5017270	-0.8030759	-4.3808167
C	1.9871035	-2.3516994	3.5226689
H	1.5582276	-4.3007657	4.3803619
H	-3.1877871	1.3615778	-4.2152931
H	2.7776628	-2.0815654	4.2125819

N	2.6142271	0.0001531	-0.0000961
C	3.2913244	0.7362922	0.8784674
C	3.2913595	-0.7360842	-0.8785523
C	4.6799440	0.7676322	0.9130002
C	2.5093134	1.5383162	1.8454321
C	4.6799793	-0.7672748	-0.9131489
C	2.5093909	-1.5382100	-1.8454620
C	5.3821877	0.0005813	-0.0003974
H	5.1837505	1.3829364	1.6449006
N	3.1677571	2.2317389	2.7693506
N	1.1921779	1.5204089	1.7387369
H	5.1838223	-1.3830964	-1.6445886
N	1.1922761	-1.5207184	-1.7384702
N	3.1678561	-2.2314639	-2.7694837
H	6.4654814	0.0011637	-0.0009307
C	2.4433446	2.9143619	3.6152309
N	0.4546292	2.1986905	2.5863617
N	0.4547411	-2.1988229	-2.5862368
C	2.4434603	-2.9141034	-3.6153723
C	1.0429184	2.8925744	3.5246699
H	2.9449455	3.4930757	4.3849562
C	1.0430349	-2.8922823	-3.5248624
H	2.9450920	-3.4928752	-4.3850265
H	0.4135467	3.4413687	4.2150951
H	0.4136625	-3.4407389	-4.2155545

B3LYP

Am	0.0005136	0.0000310	-0.0000957
N	-1.3074573	2.2636763	-0.0016200
C	-2.2954599	2.4859379	0.8834233
C	-1.0065731	3.2295734	-0.8877680
C	-3.0227086	3.6831732	0.9140379
C	-2.6033230	1.4054347	1.8540492
C	-1.6819929	4.4567475	-0.9209244
C	0.0849841	2.9568137	-1.8565771
C	-2.7068465	4.6828026	-0.0040959
H	-3.8157223	3.8099462	1.6502328
N	-3.5431803	1.6306855	2.7828621
N	-1.9198078	0.2580146	1.7443648
H	-1.3958512	5.2062084	-1.6579996
N	0.7380443	1.7919314	-1.7454592
N	0.3601753	3.8833213	-2.7853754
H	-3.2534201	5.6279043	-0.0050557
C	-3.7713847	0.6517408	3.6394174
N	-2.1367667	-0.7260346	2.6065133
N	1.7003395	1.4885161	-2.6059918
C	1.3237893	3.5923023	-3.6402823
C	-3.0425633	-0.5526056	3.5556832
H	-4.5341208	0.7981963	4.4111923
C	2.0035570	2.3597157	-3.5550017
H	1.5786927	4.3260881	-4.4119011
H	-3.1980991	-1.3758340	4.2569667
H	2.7955851	2.0833331	-4.2549800

N	-1.3075371	-2.2635036	0.0014072
C	-2.2954412	-2.4858695	-0.8837241
C	-1.0068759	-3.2292462	0.8877892
C	-3.0227002	-3.6830918	-0.9142947
C	-2.6033253	-1.4053656	-1.8543343
C	-1.6823426	-4.4563962	0.9210360
C	0.0845847	-2.9564176	1.8566726
C	-2.7070367	-4.6825788	0.0040679
H	-3.8155180	-3.8100051	-1.6506772
N	-3.5434390	-1.6304604	-2.7829322
N	-1.9198409	-0.2579263	-1.7445742
H	-1.3962878	-5.2057724	1.6582303
N	0.7382204	-1.7919160	1.7449539
N	0.3590552	-3.8824202	2.7861889
H	-3.2537855	-5.6275772	0.0052119
C	-3.7718075	-0.6514157	-3.6393235
N	-2.1365267	0.7259948	-2.6069562
N	1.7014094	-1.4889836	2.6046581
C	1.3231397	-3.5916401	3.6406474
C	-3.0424141	0.5526240	-3.5560426
H	-4.5350384	-0.7975791	-4.4106630
C	2.0045073	-2.3600383	3.5538422
H	1.5772088	-4.3248730	4.4130649
H	-3.1977196	1.3757236	-4.2575356
H	2.7974753	-2.0841852	4.2529620
N	2.6150728	0.0004552	-0.0003145
C	3.3012390	0.7434485	0.8862663
C	3.3013077	-0.7423935	-0.8869501
C	4.7016942	0.7732455	0.9183425
C	2.5187940	1.5499432	1.8568324
C	4.7017754	-0.7721230	-0.9189307
C	2.5189539	-1.5494412	-1.8571357
C	5.4096753	0.0005914	-0.0002881
H	5.2078620	1.3950001	1.6559828
N	3.1829899	2.2491435	2.7878424
N	1.1835198	1.5331110	1.7448649
H	5.2080242	-1.3940818	-1.6563423
N	1.1836905	-1.5332234	-1.7448287
N	3.1832745	-2.2485727	-2.7880997
H	6.5014407	0.0006034	-0.0003058
C	2.4484737	2.9355337	3.6442857
N	0.4390039	2.2128290	2.6064837
N	0.4393601	-2.2145751	-2.6053053
C	2.4489362	-2.9365484	-3.6434244
C	1.0411667	2.9085151	3.5577096
H	2.9558862	3.5206749	4.4182175
C	1.0416693	-2.9110205	-3.5558912
H	2.9564778	-3.5217421	-4.4172257
H	0.4053546	3.4546331	4.2585740
H	0.4059897	-3.4587065	-4.2556496

EuBTPPhen(NO₃)

BHLYP

N	1.4671952	2.8068909	1.5462735
N	2.2636185	2.6450638	0.5163853
C	1.8526777	3.0216929	-0.6672368
C	0.5717611	3.5691888	-0.8328179
N	-0.2115236	3.7339518	0.2003361
C	0.2731035	3.3522574	1.3792116
N	-0.0055949	3.2232959	3.7403896
C	-0.5531740	3.5551727	2.5887629
C	-1.8439187	4.0900566	2.4906263
H	-2.2456812	4.3476597	1.5207981
C	-2.5681449	4.2700670	3.6428883
H	-3.5731926	4.6742385	3.6041195
C	-1.9961486	3.9409038	4.8814596
C	-2.6762737	4.1325286	6.1274437
H	-3.6877938	4.5212651	6.1091633
C	-2.0652905	3.8505211	7.2996601
H	-2.5759326	4.0088505	8.2424075
C	-0.7223314	3.3519759	7.3278967
C	-0.0295381	3.1049340	8.5226668
H	-0.5211457	3.2692595	9.4746961
C	1.2754761	2.6825597	8.4753045
H	1.8516147	2.5148344	9.3741636
C	1.8663632	2.4712666	7.2237376
N	1.2177505	2.6499732	6.0887498
C	-0.0374803	3.1114606	6.1215869
C	-0.6886989	3.4171584	4.8706177
N	3.7696525	1.8427324	5.9142253
C	3.2867051	2.0707409	7.1246232
N	4.0023624	1.9894050	8.2421499
C	5.2668923	1.6887399	8.1031583
C	5.8025120	1.4765422	6.8255864
N	5.0384631	1.5489679	5.7656335
N	1.6670556	-0.3954034	5.2792007
N	0.6129401	-0.3901530	6.0601211
C	0.2652981	-1.4990074	6.6605085
C	1.0049476	-2.6749219	6.4632838
N	2.0527838	-2.6705750	5.6821520
C	2.3579144	-1.5105674	5.1064819
N	3.8210396	-0.2621589	3.7055015
C	3.5328654	-1.4439486	4.2105871
C	4.2811746	-2.5926415	3.9223868
H	4.0045860	-3.5389758	4.3655225
C	5.3515232	-2.4797420	3.0701875
H	5.9484615	-3.3487728	2.8183791
C	5.6800903	-1.2271622	2.5282638
C	6.7968542	-1.0266044	1.6537513
H	7.3963536	-1.8858006	1.3762895
C	7.1063197	0.2079821	1.1984977
H	7.9603782	0.3604855	0.5489655
C	6.3263649	1.3489239	1.5771882
C	6.6530733	2.6562862	1.1856471

H	7.5122981	2.8285926	0.5476310
C	5.8997335	3.7099778	1.6400900
H	6.1444166	4.7327668	1.3908845
C	4.7920238	3.4398772	2.4522611
C	5.1944421	1.1833739	2.3977232
C	4.8690770	-0.1339420	2.8894520
N	2.9621627	4.2173114	3.7877232
C	3.9943127	4.5456954	3.0267229
N	4.3705336	5.7964415	2.7800600
C	3.6736297	6.7390981	3.3591670
C	2.5979589	6.4071196	4.1939881
N	2.2630887	5.1551401	4.3789744
O	1.7135556	-0.0050446	2.0273545
N	0.4882354	-0.1387300	2.2096390
O	-0.0050065	0.5484449	3.1255527
O	-0.1756323	-0.8804365	1.5444800
N	4.4342679	2.2142438	2.7849772
H	5.8854508	1.6069017	8.9918346
H	6.8490838	1.2400589	6.6733560
H	-0.6075768	-1.4707392	7.3020786
H	0.7204632	-3.6025301	6.9508028
H	2.5314195	2.8863451	-1.5011041
H	0.2112171	3.8626789	-1.8141057
H	3.9446084	7.7749393	3.1785232
H	2.0092533	7.1628346	4.7007239
Eu	2.1406084	1.7335464	3.8458559

B3LYP

Eu	2.1324851	1.7250497	3.8397740
N	1.4705082	2.8252728	1.5239187
N	2.2781622	2.6763757	0.4834320
C	1.8535174	3.0610511	-0.7112319
C	0.5592644	3.5940433	-0.8776182
N	-0.2370855	3.7508100	0.1650477
C	0.2551642	3.3681099	1.3532901
N	-0.0217314	3.2209160	3.7314396
C	-0.5750344	3.5615787	2.5677710
C	-1.8762564	4.0994200	2.4727167
H	-2.2792047	4.3616516	1.4949876
C	-2.6077723	4.2780745	3.6326114
H	-3.6210116	4.6845936	3.5929938
C	-2.0330888	3.9462860	4.8802197
C	-2.7145913	4.1382818	6.1303625
H	-3.7345813	4.5289694	6.1129226
C	-2.0971828	3.8565623	7.3155039
H	-2.6136879	4.0189196	8.2642739
C	-0.7493408	3.3590027	7.3470306
C	-0.0504829	3.1157884	8.5504537
H	-0.5462104	3.2831545	9.5094914
C	1.2650026	2.6931973	8.5032299
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C	4.2865704	-2.6292507	3.9210855
H	4.0088118	-3.5823501	4.3700460
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H	0.1907136	3.8860084	-1.8665590
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AmBTPhen(NO₃)

BHLYP

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B3LYP

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C	5.7072516	-1.2650653	2.5381858
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H	0.7005246	-3.6644246	6.9722579
H	2.4898032	3.0093634	-1.5638623
H	0.1231353	3.9298641	-1.8498321
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