

Correlation of the structural information obtained for europium-chelate ensembles from gas-phase photoluminescence and ion-mobility spectroscopy with density-functional computations and ligand- field theory

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SUPPORTING INFORMATION

1. Synthesis

Mg[Eu(PLN)₄]₂ and Ca[Eu(PLN)₄]₂ are unprecedented and were prepared following a modified literature procedure of Ref. 1 using Mg(OH)₂ or Ca(OH)₂ instead of alkali metal hydroxides of sodium or potassium.

Mg[Eu(PLN)₄]₂: HPLN (0.2 g, 1 mmol, 4 eq) was dissolved in MeOH (80 mL) by gentle heating. Mg(OH)₂ (29.8 mg, 0.5 mmol, 2 eq) was added and stirred. The reaction occurred at 50°C in a water bath. After 0.5 h, finally, the Eu(H₂O)₆Cl₃ (93,4 mg, 0.255 mmol, 1 eq) was added. The reaction proceeded overnight. The solvent was removed by rotary evaporation to a small volume of about 10 mL and 3 mL of water was added to precipitate the compound as an orange powder. The remaining 5 mL of the suspension were filtered to collect the product. It was washed with 2 mL of a mixture of MeOH / water (1:1) and dried first under a stream of air and later in an oven at 120 °C. Yield 0.188g (76 %). Elemental analysis (%) calculated for M·2H₂O (C₁₀₄H₆₀Eu₂MgO₁₈, M=1925.8 g/mol): C 64.86, H 3.14; found: C 64.61, H 3.29;

Ca[Eu(PLN)₄]₂: The reaction was carried out as described above. Ca(OH)₂ was used as base. The product already precipitated without further addition of water. Yield 0.163 g (65 %) Elemental analysis (%) calculated for M·2H₂O (C₁₀₄H₆₀CaEu₂O₁₈, M=1941.6 g/mol): C 64.34, H 3.11; found: C 64.53, H 3.37.

1. Greisch, J. F.; Harding, M. E.; Schäfer, B.; Rotter, M.; Ruben, M.; Klopfer, W.; Kappes, M. M.; Schooss, D. Substitutional Photoluminescence Modulation in Adducts of a Europium Chelate with a Range of Alkali Metal Cations: A Gas-Phase Study. *J. Phys. Chem. A* **2014**, *118*, 94-102.
2. Gulde, R.; Pollak, P.; Weigend, F. Error-Balanced Segmented Contracted Basis Sets of Double- ζ to Quadruple- ζ Valence Quality for the Lanthanides. *J. Chem. Theory Comput.* **2012**, *8*, 4062-4068.
3. Weigend, F. Accurate Coulomb-Fitting Basis Sets for H to Rn. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.

2. Additional figures

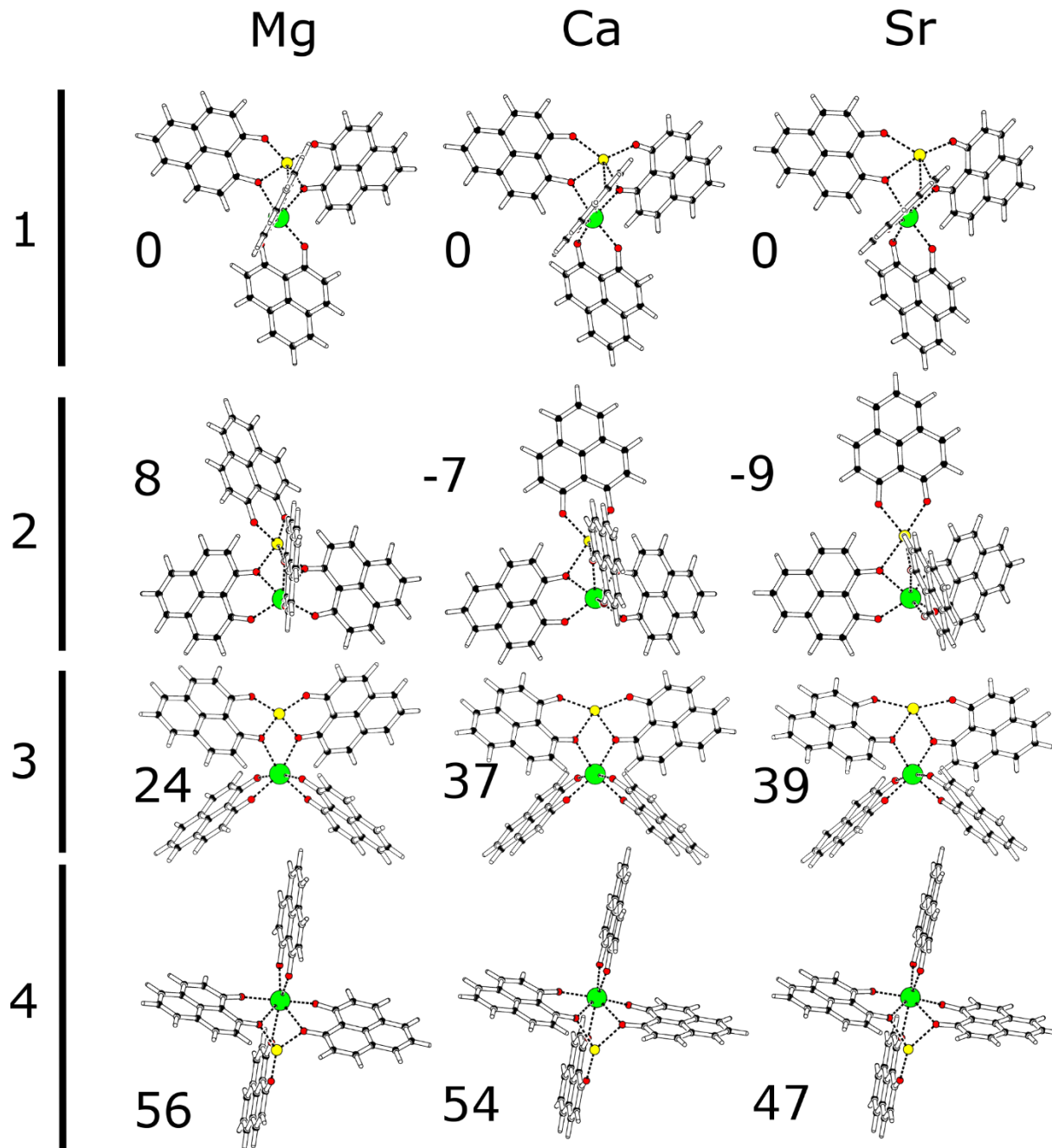


Figure SI-1. Structures computed at the RI-B-P/def2-TZVPP level. Motif 2 is lower in energy except for the species containing magnesium. Energy differences at the RI-B-P/def2-TZVPP level including harmonic zero-point corrections are given in kJ/mol. Europium: green, alkaline earth: yellow, oxygen: red.

Following the optimization at the B-P/def2-TZVPP level, the structures of motif1 and motif2 were reoptimized at the BH-LYP-D3/def2-TZVPP level. The electron densities used for population analysis were computed employing both functionals in combination with the def2-TZVPP basis set (see Figure SI-2). The resolution-of-identity (RI) approximation was applied in all calculations.²⁻³ A self-consistent-field convergence threshold of 10^{-8} Hartree and geometry convergence thresholds of 10^{-8} Hartree and 10^{-3} Hartree/Bohr for the total energy and the Cartesian gradient, respectively, were used. The numerical quadrature was performed on TURBOMOLE's grid 5.

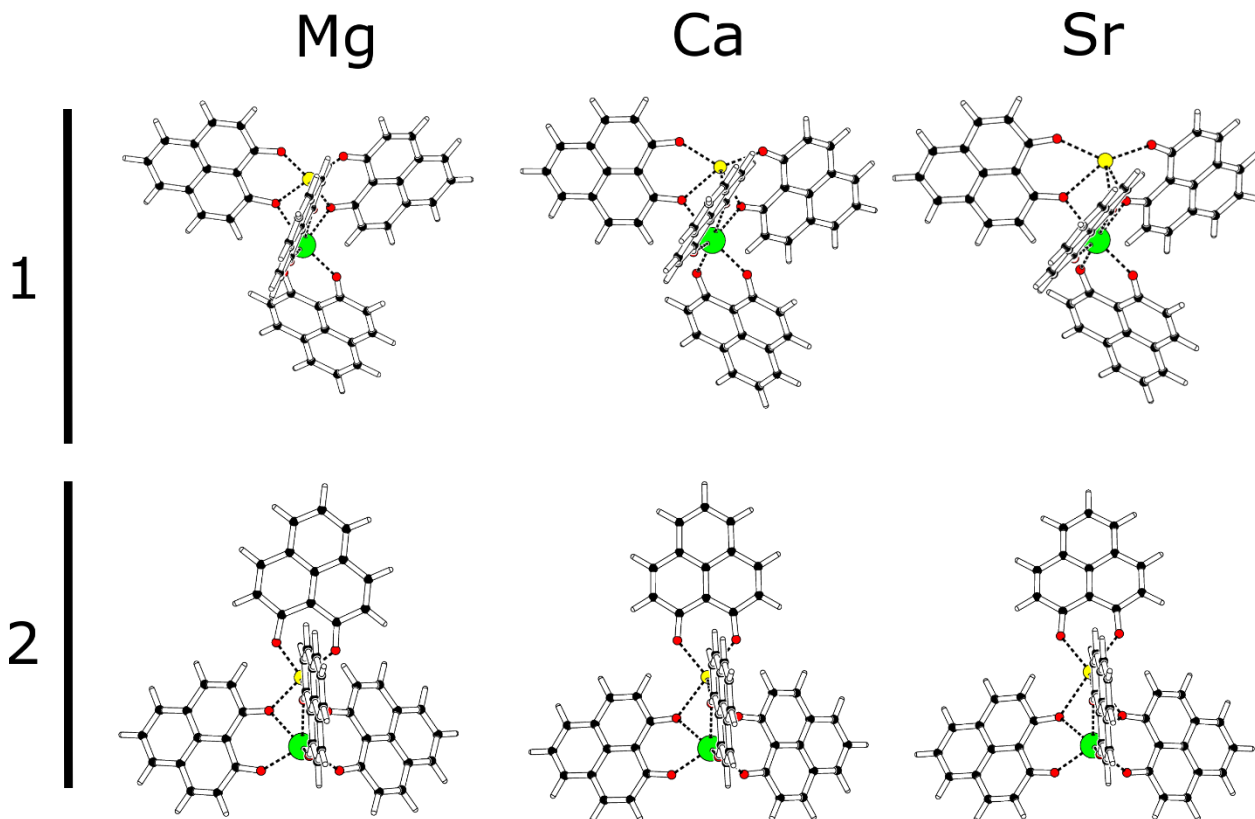


Figure SI-2. Structures computed at the BH-LYP-D3/def2-TZVPP level. Europium: green, alkaline earth: yellow, oxygen: red. The relative energies of the BH-LYP-D3 structures computed at the BH-LYP-D3/def2-TZVPP level (1, -9, and -5 kJ/mol) are in line with those previously computed at the B-P-D3/def2-TZVPP level (8, -6, and -8 kJ/mol) at the B-P minimum geometries and those obtained at the B2PLYP/def2-TZVPP level (1, -12, and -11 kJ/mol) at the B-P minimum geometries.

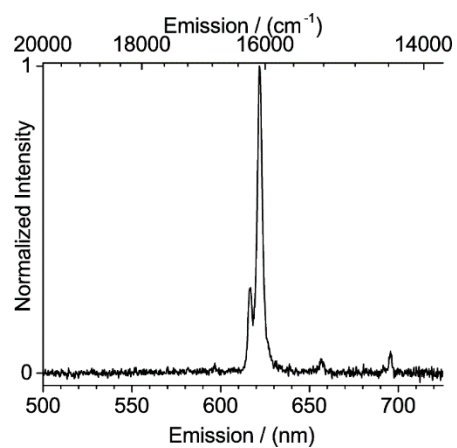


Figure SI-3. Spectrum of [Eu(PLN)₄Mg]⁺ taken at 85K under 1340 W/cm² excitation at 458 nm and about 0.2 mbar He buffer gas pressure ($q_z \sim 0.8$). Spectral resolution 2.4 nm.

Table SI-1. Absolute ${}^5D_0 \rightarrow {}^7F_2$ transitions of $[\text{Eu}(\text{PLN})_4\text{AE}]^+$ with AE = Mg, Ca, and Sr. The experimental transitions

$[\text{Eu}(\text{PLN})_4\text{Mg}^+]$ \ [cm ⁻¹]	Exp.	motif 1	line(x)- line(x+1)	motif 2	line(x)- line(x+1)	motif 3	line(x)- line(x+1)	motif 4	line(x)- line(x+1)
${}^5D_0 \rightarrow {}^7F_2(a)$	16218	16307	29	16266	35	17804	68	16412	53
${}^5D_0 \rightarrow {}^7F_2(b)$		16278		16231		17736		16359	
${}^5D_0 \rightarrow {}^7F_2(c)$	16079	16229	131	16214	89	17082	59	16146	41
${}^5D_0 \rightarrow {}^7F_2(d)$		16098		16125		17023		16105	
${}^5D_0 \rightarrow {}^7F_2(e)$		16058		16098		15908		15972	

$[\text{Eu}(\text{PLN})_4\text{Ca}^+]$ \ [cm ⁻¹]	Exp.	motif 1	line(x)- line(x+1)	motif 2	line(x)- line(x+1)	motif 3	line(x)- line(x+1)	motif 4	line(x)- line(x+1)
${}^5D_0 \rightarrow {}^7F_2(a)$	16236	16306	39	16251	16	17689	607	16412	53
${}^5D_0 \rightarrow {}^7F_2(b)$		16267		16235		17082		16359	
${}^5D_0 \rightarrow {}^7F_2(c)$	16090	16234	141	16194	66	16973	109	16145	214
${}^5D_0 \rightarrow {}^7F_2(d)$		16093		16128		15912		1061	
${}^5D_0 \rightarrow {}^7F_2(e)$		16069		16121		14558		15975	

$[\text{Eu}(\text{PLN})_4\text{Sr}^+]$ \ [cm ⁻¹]	Exp.	motif 1	line(x)- line(x+1)	motif 2	line(x)- line(x+1)	motif 3	line(x)- line(x+1)	motif 4	line(x)- line(x+1)
${}^5D_0 \rightarrow {}^7F_2(a)$	16243	16305	44	16248	9	17654	590	16375	41
${}^5D_0 \rightarrow {}^7F_2(b)$		16261		16239		17064		16334	
${}^5D_0 \rightarrow {}^7F_2(c)$	16093	16236	137	16190	49	16938	126	16155	179
${}^5D_0 \rightarrow {}^7F_2(d)$		16099		16128		15914		1024	
${}^5D_0 \rightarrow {}^7F_2(e)$		16066		16124		14562		16005	

3. Computed hypersensitive transitions maps

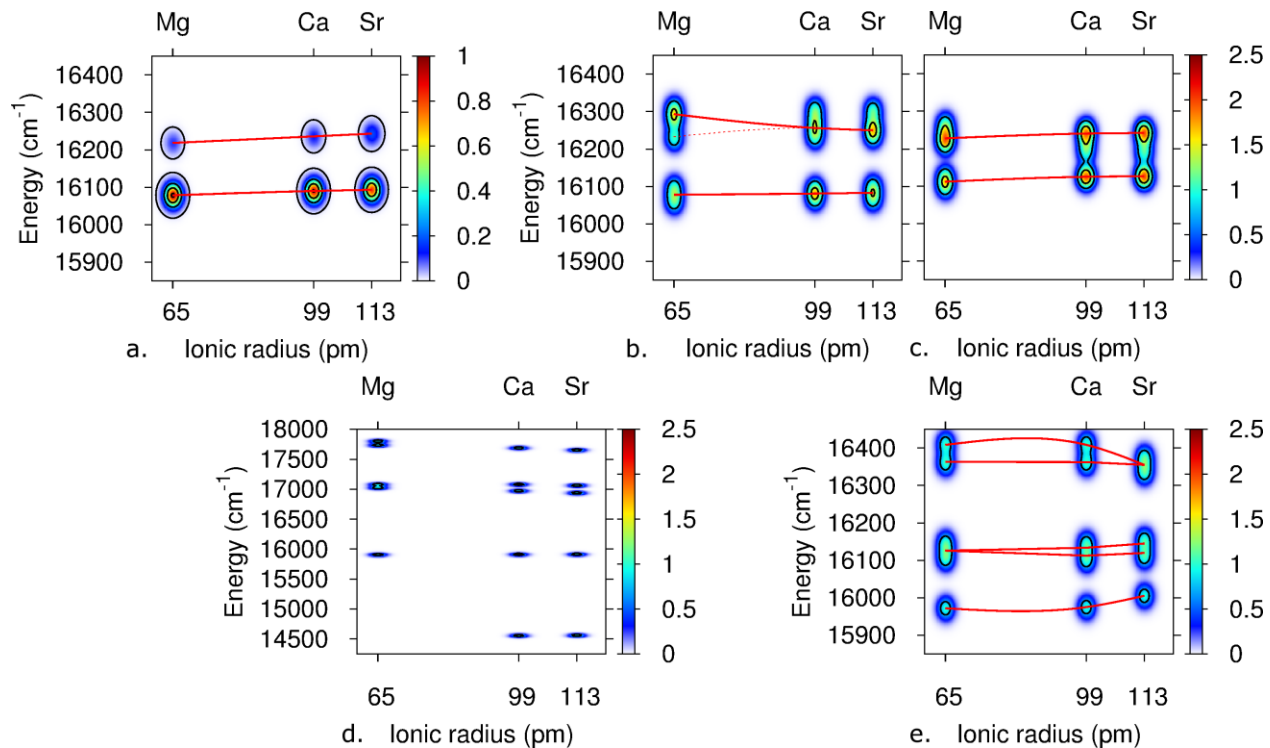


Figure SI-4. a) Experimental band positions and relative intensities for the ${}^5D_0 \rightarrow {}^7F_2$ transitions of $[\text{Eu}(\text{PLN})_4\text{AE}]^+$ with AE = Mg, Ca, and Sr. b-e) Splitting of the 7F_2 level calculated using McPHASE for the motif 1 (b), motif 2 (c), motif 3 (d), and motif 4 (e) geometries (see text). Red lines are used to highlight trends. Absolute values of the computed transitions in table SI-1.

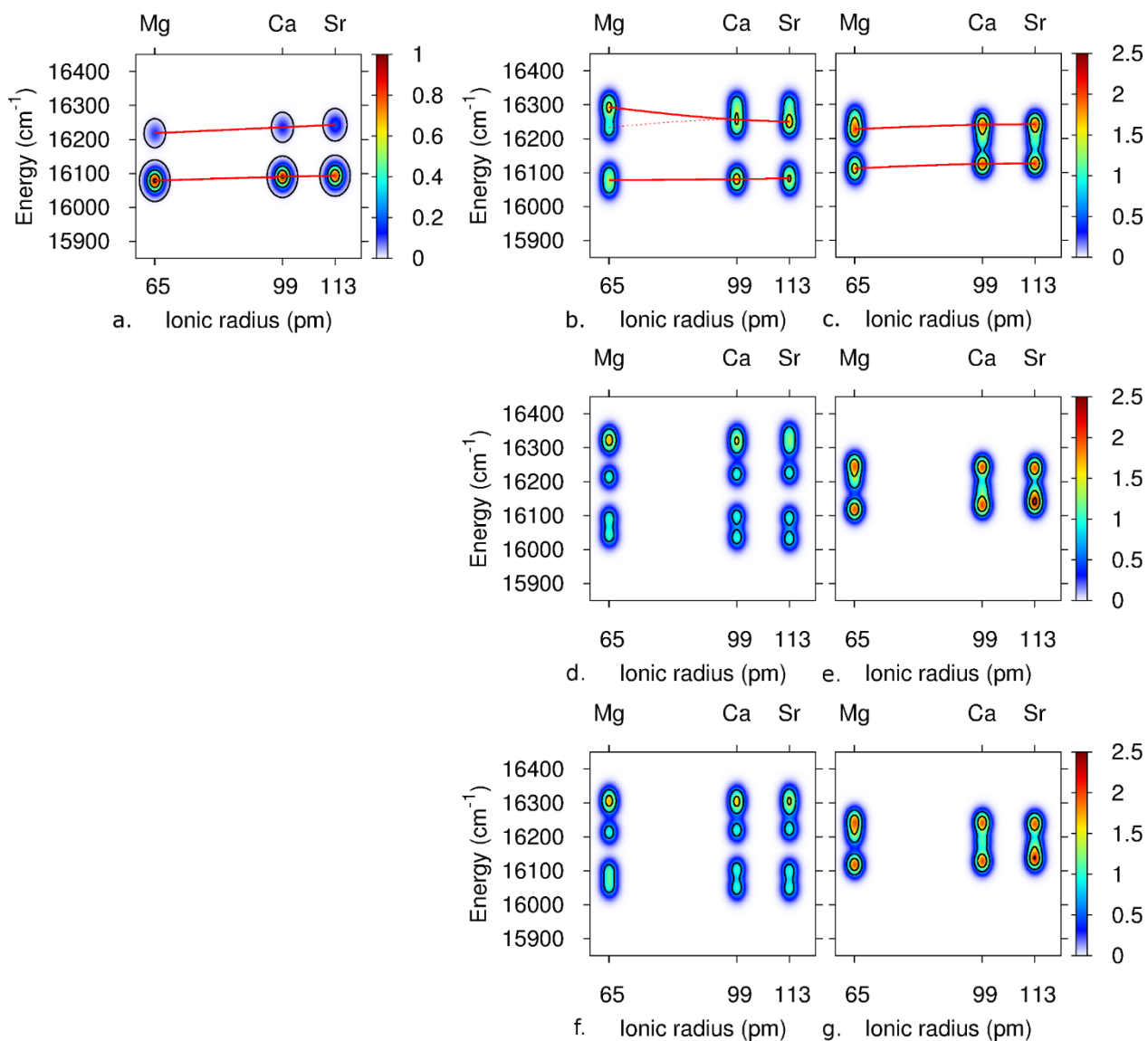


Figure SI-5. Band positions and relative intensities for the ${}^5D_0 \rightarrow {}^7F_2$ transitions of $[\text{Eu}(\text{PLN})_4\text{AE}]^+$ with AE = Mg, Ca, and Sr. a. corresponds to the experiment, b-c. to B-P, d-e to BHLYP-D3, and f-g. to BP@BHLYP-D3. As already can be seen for the structures the change from B-P to BH-LYP-D3 has almost no impact on our results. Again motif 2 is probably favored.

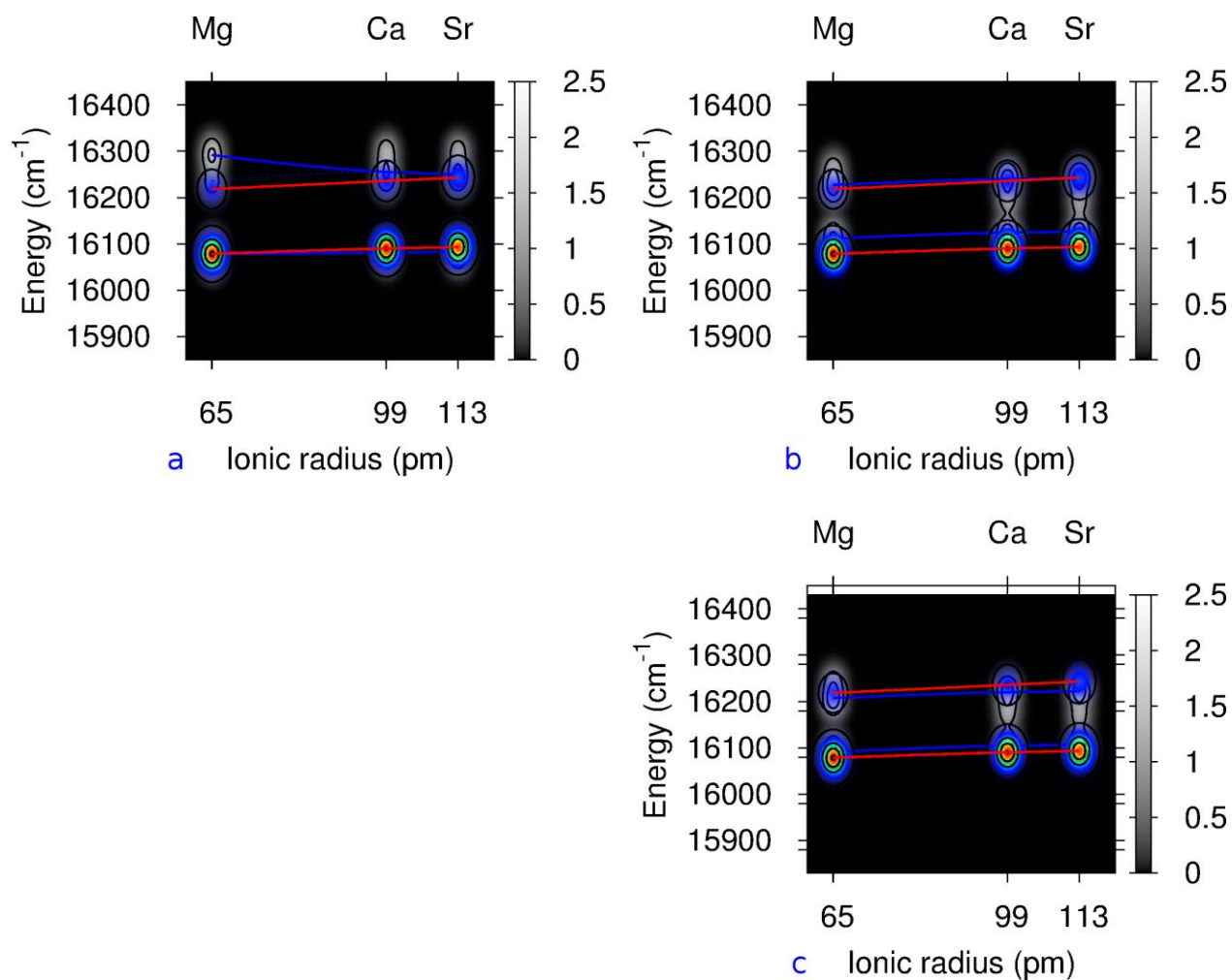


Figure SI-6. Superposition of the experimental band positions (highlighted by red lines) and relative intensities for the ${}^5D_0 \rightarrow {}^7F_2$ transitions of $[\text{Eu}(\text{PLN})_4\text{AE}]^+$ with AE = Mg, Ca, and Sr on the computed transitions from the 5D_0 level to the split 7F_2 levels manifold calculated using McPHASE for the motif 1 (a), motif 2 (b and c) geometries. (c) corresponds to a systematic shift of the computed transitions by about -20 cm^{-1} (down shift of $\sim 20 \text{ cm}^{-1}$).

4. Structures

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[Eu(PLN)4Mg]+, motif 1, RI-B-P/def2-TZVPP
Energy = -3512.485569564
Eu   -0.0479474   -0.8073114    0.2598808
Mg   -0.0286808    2.3323507   -0.2223712
C    -0.7718150   -3.7067781   -1.2445605
C    -0.5168753   -4.5151633   -2.4057803
H     0.0718490   -4.0593786   -3.2009334
C    -1.0025624   -5.7884689   -2.5114144
H    -0.7975125   -6.3788691   -3.4064774
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C	-1.7844209	-6.3764103	-1.4707903
C	-2.0477477	-5.6084541	-0.2942614
C	-1.5367835	-4.2802128	-0.1581714
C	-2.2912750	-7.6851760	-1.5809028
H	-2.0755533	-8.2572031	-2.4845885
C	-3.0567708	-8.2505764	-0.5620959
H	-3.4429117	-9.2637223	-0.6644983
C	-3.3259101	-7.5101523	0.5879828
H	-3.9275112	-7.9427848	1.3887817
C	-2.8338118	-6.1999949	0.7422265
C	-3.1077480	-5.4323637	1.9141501
H	-3.7132872	-5.8823679	2.7031035
C	-2.6265914	-4.1610985	2.0628004
H	-2.8290000	-3.5774337	2.9598673
C	-1.8097612	-3.5442944	1.0554068
C	-1.0451682	3.2760132	-2.8588768
C	-1.0968792	4.3690630	-3.7967911
H	-0.4961757	5.2444068	-3.5520836
C	-1.8680084	4.3188186	-4.9201432
H	-1.8943390	5.1671209	-5.6068876
C	-2.6602686	3.1679140	-5.2279618
C	-2.6279787	2.0518525	-4.3360375
C	-1.8253012	2.0810823	-3.1474190
C	-3.4565878	3.1201253	-6.3845360
H	-3.4647149	3.9844975	-7.0504327
C	-4.2274808	1.9958826	-6.6899303
H	-4.8396158	1.9789902	-7.5905345
C	-4.2037020	0.9001135	-5.8352989
H	-4.7984091	0.0137227	-6.0614478
C	-3.4154314	0.9062698	-4.6641447
C	-3.3797341	-0.2152872	-3.7888142
H	-3.9812273	-1.0925001	-4.0338281
C	-2.6093381	-0.2065044	-2.6571382
H	-2.5828245	-1.0716025	-1.9951450
C	-1.8130324	0.9250872	-2.2945921
O	-0.3162879	-2.4990484	-1.2342654
O	-1.3514218	-2.3560922	1.2852296
O	-0.3164716	3.4235511	-1.8148032
O	-1.1086350	0.8511102	-1.1877483
C	3.2734252	-1.1313891	0.7454974
C	4.2491843	-2.0654525	1.2373352
H	3.8650552	-2.9733369	1.7008476
C	5.5896654	-1.8304188	1.1220743
H	6.3083355	-2.5616003	1.4970557
C	6.0849989	-0.6352737	0.5162762
C	5.1481954	0.3257196	0.0262932
C	3.7370497	0.0940882	0.1248202
C	7.4661581	-0.3909506	0.4035884
H	8.1630895	-1.1394001	0.7838388
C	7.9488617	0.7817886	-0.1775680
H	9.0212971	0.9537852	-0.2567842
C	7.0480629	1.7317168	-0.6504703
H	7.4120892	2.6562867	-1.1010495
C	5.6561137	1.5262488	-0.5571117

C	4.7289009	2.5001502	-1.0274499
H	5.1132035	3.4189318	-1.4739082
C	3.3783702	2.3001352	-0.9307177
H	2.6765178	3.0480152	-1.3017326
C	2.8349371	1.1002985	-0.3691502
C	0.2295254	3.8921924	2.3273110
C	0.6159871	5.1504639	2.9175532
H	1.0298456	5.8952952	2.2387885
C	0.4598979	5.3990272	4.2484245
H	0.7538837	6.3642988	4.6651688
C	-0.0893265	4.4149535	5.1319523
C	-0.4770450	3.1476677	4.5956215
C	-0.3274187	2.8641979	3.1997731
C	-0.2457530	4.6726667	6.5028167
H	0.0567917	5.6464225	6.8910832
C	-0.7765282	3.7104538	7.3675381
H	-0.8909975	3.9312259	8.4278397
C	-1.1543445	2.4719915	6.8634389
H	-1.5678295	1.7112756	7.5272170
C	-1.0130567	2.1708754	5.4913004
C	-1.3949231	0.9038278	4.9672842
H	-1.8080498	0.1571467	5.6477043
C	-1.2565116	0.6172290	3.6352098
H	-1.5635207	-0.3510539	3.2361626
C	-0.7243944	1.5733673	2.7127450
O	2.0286858	-1.4342315	0.8862993
O	1.5332956	0.9743821	-0.3355762
O	0.3934141	3.7488123	1.0681140
O	-0.6334770	1.2194465	1.4508207

[Eu(PLN)₄Mg]⁺, motif 2, RI-B-P/def2-TZVPP

Energy = -3512.482442423

Eu	0.4060889	-1.6023552	-2.1378279
Mg	-0.2052191	0.2736509	0.4069387
C	-0.9662308	-4.4596440	-0.9535125
C	-1.1446035	-5.8500992	-1.2765031
H	-0.7014322	-6.1933564	-2.2105575
C	-1.8378660	-6.6929200	-0.4575004
H	-1.9609056	-7.7435017	-0.7271479
C	-2.4204522	-6.2286285	0.7625714
C	-2.2618651	-4.8542106	1.1241833
C	-1.5310156	-3.9516521	0.2848425
C	-3.1398729	-7.0970305	1.6016782
H	-3.2464920	-8.1418226	1.3060296
C	-3.7128720	-6.6460682	2.7923481
H	-4.2673477	-7.3340997	3.4288923
C	-3.5700766	-5.3112508	3.1571403
H	-4.0141872	-4.9447358	4.0837972
C	-2.8543091	-4.4072109	2.3451089
C	-2.7066581	-3.0393851	2.7105742
H	-3.1635858	-2.6905184	3.6381751
C	-2.0068936	-2.1663039	1.9227039
H	-1.9012020	-1.1224913	2.2169590
C	-1.3891781	-2.5797058	0.6994908

C	-1.4962710	1.3047791	-2.4130342
C	-2.1175916	2.4155233	-1.7523167
H	-2.0053312	2.4696051	-0.6692351
C	-2.8241338	3.3613385	-2.4414353
H	-3.2772699	4.1985902	-1.9069888
C	-2.9897279	3.2856185	-3.8546061
C	-2.4044466	2.1830567	-4.5491509
C	-1.6597246	1.1789631	-3.8469582
C	-3.7178802	4.2618668	-4.5612417
H	-4.1567385	5.0919748	-4.0056162
C	-3.8820035	4.1797001	-5.9424174
H	-4.4466259	4.9431743	-6.4756464
C	-3.3173722	3.1103131	-6.6354936
H	-3.4385359	3.0341027	-7.7170467
C	-2.5847265	2.1115919	-5.9667499
C	-2.0088263	1.0185998	-6.6815858
H	-2.1475760	0.9694362	-7.7631097
C	-1.2970616	0.0497950	-6.0346162
H	-0.8553093	-0.7911560	-6.5676388
C	-1.1015549	0.0835917	-4.6119324
O	-0.3164743	-3.7273703	-1.7849886
O	-0.7251195	-1.6848645	0.0088617
O	-0.8053372	0.4685241	-1.6844069
O	-0.4306704	-0.8803050	-4.0803050
C	2.8212696	0.2746825	-0.4551516
C	3.0944091	1.3000017	0.5072377
H	2.2503809	1.7082893	1.0604322
C	4.3636492	1.7487324	0.7481326
H	4.5325645	2.5341250	1.4869034
C	5.4838972	1.2071258	0.0553481
C	5.2538670	0.1859110	-0.9162511
C	3.9286063	-0.2848985	-1.1928180
C	6.7943296	1.6573628	0.3124431
H	6.9427945	2.4394405	1.0585268
C	7.8855438	1.1206671	-0.3656814
H	8.8929805	1.4770388	-0.1557982
C	7.6770879	0.1223250	-1.3170714
H	8.5243721	-0.3058268	-1.8547518
C	6.3846894	-0.3527824	-1.6063056
C	6.1743347	-1.3700809	-2.5864793
H	7.0411196	-1.7800476	-3.1080812
C	4.9196940	-1.8217875	-2.8789855
H	4.7472600	-2.5912712	-3.6304167
C	3.7579677	-1.3021643	-2.2114030
C	0.3438649	0.6281745	3.3334588
C	1.1372532	0.2595652	4.4795385
H	1.9432862	-0.4527399	4.3050290
C	0.8902289	0.7731539	5.7201140
H	1.5071855	0.4749213	6.5702470
C	-0.1713521	1.7054488	5.9436099
C	-0.9827236	2.0983082	4.8340810
C	-0.7398071	1.5717658	3.5253492
C	-0.4265426	2.2361727	7.2210828
H	0.2048020	1.9241718	8.0546388

C	-1.4633790	3.1454177	7.4320005
H	-1.6465378	3.5465972	8.4278862
C	-2.2620996	3.5371059	6.3596627
H	-3.0753390	4.2481693	6.5136006
C	-2.0409166	3.0309568	5.0641226
C	-2.8532454	3.4266350	3.9582701
H	-3.6640499	4.1362376	4.1345197
C	-2.6325513	2.9354254	2.7021081
H	-3.2557501	3.2344356	1.8597521
C	-1.5758334	1.9987176	2.4276874
O	1.5784913	-0.0960575	-0.6260076
O	2.6083345	-1.7633426	-2.5609513
O	0.6381393	0.1016226	2.1977982
O	-1.4335663	1.5871210	1.2075927

[Eu(PLN)₄Mg]⁺, motif 3, RI-B-P/def2-TZVPP

Energy = -3512.476238844

H	-6.6167304	2.5129484	5.0910749
H	-7.1767004	1.2708666	3.0077615
C	-5.8282021	2.2251011	4.3971364
C	-6.1400796	1.5283936	3.2305596
H	-6.4896721	0.1844432	0.9182204
H	-4.2464033	3.0939370	5.5812698
C	-4.5003198	2.5504181	4.6698451
C	-5.1362498	1.1432292	2.3218538
C	-5.4459636	0.4301891	1.1236310
C	-3.4656444	2.1894112	3.7860804
C	-3.7710777	1.4711146	2.5888069
C	-4.4691266	0.0538377	0.2449176
H	-4.7014374	-0.4964592	-0.6661168
H	-1.8697536	3.0608836	4.9753041
C	-2.1024035	2.5190236	4.0564814
C	-2.7352722	1.0887771	1.6806420
C	-3.0824006	0.3459833	0.4903227
C	-1.1003154	2.1708073	3.1945461
C	-1.3691833	1.4587435	1.9744561
H	3.0519530	-3.0173016	-7.9584138
H	2.6422304	-0.6641747	-7.2661219
O	-2.2132046	-0.0781015	-0.3649090
H	2.7011824	-5.4078948	-7.6286463
C	2.4449850	-2.7949434	-7.0787839
H	-3.0615539	6.2012073	-5.4861728
C	2.2285918	-1.5009688	-6.7045863
H	-2.6125546	3.8266534	-6.0733813
C	2.0958381	-5.2167561	-6.7412437
H	-2.7555179	8.1006910	-3.9886001
C	1.8820890	-3.8857385	-6.3447746
C	-2.4529277	5.5731002	-4.8329892
H	-0.0596435	2.4215528	3.3973017
C	-2.2147801	4.2706636	-5.1616442
H	1.7246169	-7.3092016	-6.3501044
C	1.4159894	-1.1681386	-5.5658820
C	1.5509516	-6.2847525	-6.0240458
C	-2.1486410	7.4958882	-3.3130485

O	1.2093647	0.0790579	-5.3278310
C	-1.9114243	6.1504838	-3.6419258
O	-1.1758981	2.2242841	-4.7595842
C	1.0967539	-3.6037355	-5.1851257
C	-1.4002523	3.4188017	-4.3379371
C	0.8636363	-2.2518791	-4.7638545
H	-1.8173022	9.1079775	-1.9128712
C	-1.6252157	8.0621587	-2.1480941
C	0.7889719	-6.0274634	-4.8909905
C	-1.1234136	5.3319893	-2.7757243
O	-0.3754726	1.1882278	1.1959894
Mg	0.0163672	0.8885370	-4.0485282
C	0.5558624	-4.7046332	-4.4538997
C	-0.8668522	3.9560910	-3.0931974
H	0.3590009	-6.8510239	-4.3190121
C	-0.8605643	7.2783209	-1.2927949
C	0.1073720	-2.0298975	-3.5631040
C	-0.6038066	5.9199029	-1.5826053
O	-0.1250654	-0.8275748	-3.0587272
C	-0.2119049	-4.4353437	-3.2875192
H	-0.4469484	7.7054662	-0.3780505
C	-0.1071994	3.1686668	-2.1622486
C	-0.4211736	-3.1510559	-2.8571113
O	0.1467185	1.8801346	-2.3324606
C	0.1673821	5.1092762	-0.7048636
H	-0.6354894	-5.2729614	-2.7309017
C	0.4003792	3.7872567	-0.9812041
H	-1.0060406	-2.9523427	-1.9594067
H	0.5747021	5.5564751	0.2034100
H	0.9874066	3.1713828	-0.3003107
Eu	0.0481020	-0.0190669	-0.6845358
O	2.3234778	-0.0912058	-0.4895870
H	4.7961430	0.4719761	-0.6452572
O	0.5552704	-2.0123361	0.2844108
C	3.2310572	-0.8800475	-0.0201281
C	4.6059893	-0.4761896	-0.1436632
C	1.5855356	-2.6316643	0.7550160
C	2.9384799	-2.1389430	0.6271206
C	5.6230992	-1.2358436	0.3625564
H	6.6570612	-0.8991649	0.2651806
H	0.3420663	-4.2178713	1.5321707
C	1.3733414	-3.8795739	1.4373995
C	4.0161152	-2.9186111	1.1511507
C	5.3687938	-2.4741668	1.0274174
C	2.4154483	-4.6077643	1.9394581
C	3.7660933	-4.1606978	1.8125568
C	6.4144860	-3.2572556	1.5518073
H	7.4406041	-2.9018459	1.4454751
H	2.2255217	-5.5531307	2.4514971
C	4.8415993	-4.9098805	2.3262844
C	6.1566729	-4.4653433	2.1980791
H	4.6299426	-5.8532361	2.8321128
H	6.9772363	-5.0576510	2.6006154

[Eu(PLN)₄Mg]⁺, motif 4, RI-B-P/def2-TZVPP

Energy = -3512.464052351

H	7.4065258	-1.7045221	2.2593008
H	9.1168847	-1.3656373	0.4830454
H	5.0683837	-1.7152018	2.9982960
C	7.1017172	-1.4080384	1.2544942
C	8.0607974	-1.2197027	0.2601252
C	4.7418636	-1.4182719	1.9997640
C	5.7324092	-1.2230385	0.9887760
C	7.6601921	-0.8442160	-1.0223222
H	8.4047456	-0.6946425	-1.8057196
H	2.6540649	-1.3843812	2.5059073
C	3.4129634	-1.2409033	1.7375881
C	5.3070962	-0.8383790	-0.3219608
C	6.3022948	-0.6523152	-1.3332597
H	0.2375187	-6.5512350	-3.4517657
H	0.7988818	-4.1545366	-3.7995948
C	2.9481190	-0.8346763	0.4375508
C	3.9232223	-0.6453241	-0.6140815
C	5.8836293	-0.2667542	-2.6451621
H	6.6463181	-0.1233297	-3.4130551
C	-0.1656969	-5.7845248	-2.7873103
C	0.1476022	-4.4720459	-2.9862233
H	-0.9224492	-8.2907428	-2.1918996
O	1.6812171	-0.6569995	0.2758857
C	3.5308975	-0.2701459	-1.9593881
C	4.5653339	-0.0793302	-2.9452682
C	-1.3448517	-7.5456954	-1.5158799
C	-1.0203303	-6.1932159	-1.7150975
C	-0.3468041	-3.4340883	-2.1163035
O	0.0221605	-2.2310567	-2.3447679
H	0.0544757	7.9919791	3.0712727
H	-1.2464981	6.0917111	4.0176304
O	2.3111233	-0.1036808	-2.3192771
H	4.2404485	0.2088756	-3.9443794
C	-0.0170980	7.0506829	2.5282621
C	-0.7409968	5.9884036	3.0562977
H	-2.1051646	3.8005590	3.8475604
H	1.1698362	7.7374594	0.8590340
C	0.6109623	6.9045791	1.2886413
C	-0.8443701	4.7617436	2.3642081
C	-1.6043660	3.6780170	2.8856326
C	0.5363121	5.7002058	0.5693572
C	-1.7140939	2.4971819	2.1992208
C	-0.1894221	4.5922435	1.1060673
H	-2.2924895	1.6672523	2.6070789
H	-2.4322854	-8.9976491	-0.3419814
C	-2.1938827	-7.9440939	-0.4804473
H	1.7069503	6.4123553	-1.1186522
C	1.1619853	5.5590761	-0.7100222
C	-1.0558000	2.2879053	0.9474665
C	-0.2702942	3.3512753	0.3932201
C	-1.5582700	-5.1950136	-0.8453101
C	-1.2337681	-3.8108146	-1.0257325

O	-1.2092473	1.1219803	0.3592692
C	1.0907363	4.3919062	-1.4115444
C	0.4076301	3.2324901	-0.8911274
Eu	0.2230069	-0.1441197	-1.3824749
H	1.5693636	4.2765424	-2.3832835
O	0.4373915	2.1577591	-1.5815011
C	-2.7373386	-6.9839620	0.3650756
C	-2.4384393	-5.6141956	0.1987369
C	-1.8285484	-2.8418294	-0.1516628
O	-2.2721994	0.3786846	-2.2126525
O	-1.5975858	-1.5518517	-0.2385891
H	-1.4825201	0.7659229	-4.5904534
Mg	-2.7205333	0.0669774	-0.3109914
H	-3.4101623	-7.2794199	1.1715032
C	-3.0991669	0.7183927	-3.1606116
C	-2.5557922	0.9129037	-4.4720387
C	-3.0070332	-4.6226668	1.0460318
C	-2.7217030	-3.2944774	0.8699063
O	-4.5755282	0.3996506	-0.5742121
H	-3.6795852	-4.9360736	1.8463301
H	-3.1539587	-2.5422005	1.5313774
C	-3.3387595	1.2693817	-5.5336085
H	-2.8934730	1.4104259	-6.5200882
C	-4.5211806	0.9055722	-2.9589065
C	-5.1776819	0.7335892	-1.6742241
C	-4.7423040	1.4645418	-5.3815296
C	-5.3251737	1.2800785	-4.0898878
H	-7.0481634	0.8040193	-0.6106908
C	-6.5950145	0.9434740	-1.5915414
H	-5.0752504	1.9661346	-7.4519385
C	-5.5480010	1.8324548	-6.4777124
C	-6.7342333	1.4802802	-3.9597013
C	-7.3384471	1.3002065	-2.6797252
H	-8.4148561	1.4535342	-2.5830018
C	-6.9192924	2.0242921	-6.3332378
C	-7.5033534	1.8479275	-5.0802341
H	-7.5290353	2.3087332	-7.1895326
H	-8.5768674	1.9943377	-4.9512486

[Eu(PLN)₄Ca]⁺, motif 1, RI-B-P/def2-TZVPP

Energy = -3990.071380082

Eu	0.0985398	-0.5170280	0.1717165
Ca	0.3058901	2.8176743	-0.4328187
C	-0.4854147	-3.4579880	-1.3266345
C	-0.1027226	-4.3067237	-2.4224278
H	0.6040258	-3.8922129	-3.1402234
C	-0.6113990	-5.5675843	-2.5617784
H	-0.3062479	-6.1892120	-3.4057534
C	-1.5462047	-6.1026775	-1.6234739
C	-1.9426439	-5.2931909	-0.5145522
C	-1.4134977	-3.9754849	-0.3444806
C	-2.0754597	-7.3989521	-1.7688118
H	-1.7575246	-8.0031771	-2.6198719
C	-2.9900522	-7.9124624	-0.8500527

H	-3.3908037	-8.9169232	-0.9786398
C	-3.3883455	-7.1315728	0.2333487
H	-4.1057309	-7.5234096	0.9560224
C	-2.8800724	-5.8313229	0.4197489
C	-3.2842583	-5.0220903	1.5238894
H	-4.0047720	-5.4311950	2.2346662
C	-2.7876647	-3.7605992	1.7036912
H	-3.0927540	-3.1442010	2.5483492
C	-1.8270437	-3.1948863	0.7982215
C	-1.3333327	3.3577375	-3.2167404
C	-1.5925912	4.3438262	-4.2364469
H	-1.0376787	5.2779963	-4.1556182
C	-2.4921479	4.1287196	-5.2371673
H	-2.6733644	4.8982996	-5.9900683
C	-3.2224795	2.9024143	-5.3257938
C	-2.9883774	1.8865572	-4.3466348
C	-2.0405962	2.0841886	-3.2856703
C	-4.1546789	2.6890696	-6.3552129
H	-4.3122019	3.4807471	-7.0894020
C	-4.8723996	1.4950242	-6.4504795
H	-5.5918943	1.3493400	-7.2549547
C	-4.6575488	0.4960096	-5.5083179
H	-5.2093489	-0.4434247	-5.5675250
C	-3.7279719	0.6691721	-4.4609257
C	-3.5036883	-0.3537484	-3.4977216
H	-4.0715026	-1.2827184	-3.5747099
C	-2.5943968	-0.1869345	-2.4900745
H	-2.4292174	-0.9799782	-1.7606610
C	-1.8267980	1.0146642	-2.3422520
O	0.0097625	-2.2675547	-1.2794067
O	-1.3744246	-2.0085668	1.0516932
O	-0.4980167	3.6587061	-2.2950210
O	-0.9707049	1.0699509	-1.3510088
C	3.3303019	-1.0020296	1.0094168
C	4.1897423	-1.8752469	1.7630049
H	3.7004093	-2.6310364	2.3761737
C	5.5496284	-1.7731003	1.6987938
H	6.1782773	-2.4575253	2.2715970
C	6.1838239	-0.7826543	0.8865733
C	5.3664505	0.1201234	0.1390853
C	3.9366665	0.0315787	0.1907596
C	7.5849486	-0.6807697	0.8198415
H	8.1888449	-1.3798057	1.4005046
C	8.2050716	0.2911307	0.0329819
H	9.2915601	0.3531550	-0.0071460
C	7.4230477	1.1812839	-0.6956597
H	7.8940570	1.9487938	-1.3116129
C	6.0142724	1.1158649	-0.6539906
C	5.2075216	2.0287781	-1.3903436
H	5.6968248	2.7832713	-2.0087950
C	3.8407627	1.9683414	-1.3354337
H	3.2332882	2.6590794	-1.9225071
C	3.1548055	0.9860962	-0.5487847
C	0.3279533	4.1515609	2.5807477

C	0.6427243	5.3567264	3.3092067
H	1.0586278	6.1776281	2.7259328
C	0.4195442	5.4697862	4.6484586
H	0.6601564	6.3979305	5.1705487
C	-0.1351605	4.3877584	5.4026931
C	-0.4520658	3.1665093	4.7284601
C	-0.2236122	3.0194314	3.3198589
C	-0.3645884	4.5101947	6.7826675
H	-0.1125205	5.4517078	7.2731212
C	-0.9037816	3.4576130	7.5267416
H	-1.0761335	3.5734691	8.5958278
C	-1.2170033	2.2632844	6.8889913
H	-1.6387489	1.4316785	7.4555110
C	-0.9994388	2.0976559	5.5044775
C	-1.3196326	0.8763158	4.8484434
H	-1.7463806	0.0608080	5.4351174
C	-1.1050440	0.7175168	3.5065313
H	-1.3697320	-0.2184836	3.0108078
C	-0.5473354	1.7612244	2.6968987
O	2.0607247	-1.1858207	1.0940746
O	1.8461872	1.0182886	-0.5439805
O	0.5430223	4.1395518	1.3215762
O	-0.3683124	1.5080581	1.4228119

[Eu(PLN)₄Ca]⁺, motif 2, RI-B-P/def2-TZVPP
Energy = -3990.073770235

Eu	0.4074509	-1.5375891	-2.1376481
Ca	-0.2207383	0.3516528	0.6692029
C	-0.7980627	-4.5457288	-1.1831718
C	-0.8387146	-5.9250653	-1.5902104
H	-0.3616115	-6.1663849	-2.5392688
C	-1.4527864	-6.8784086	-0.8311967
H	-1.4734479	-7.9173051	-1.1656223
C	-2.0824067	-6.5478745	0.4086956
C	-2.0568605	-5.1896454	0.8549732
C	-1.4118871	-4.1719111	0.0786000
C	-2.7177101	-7.5313881	1.1872952
H	-2.7223179	-8.5613718	0.8274603
C	-3.3347920	-7.2117475	2.3976780
H	-3.8228131	-7.9873356	2.9861197
C	-3.3213636	-5.8941955	2.8446606
H	-3.8016591	-5.6294907	3.7877993
C	-2.6923878	-4.8781119	2.0961287
C	-2.6781359	-3.5274536	2.5464708
H	-3.1697366	-3.2815981	3.4892631
C	-2.0632491	-2.5461122	1.8181402
H	-2.0698448	-1.5156508	2.1774164
C	-1.3988014	-2.8198967	0.5773875
C	-1.4127891	1.4168117	-2.4045840
C	-1.9370886	2.5731669	-1.7370015
H	-1.7419516	2.6735522	-0.6680221
C	-2.6857739	3.5104094	-2.3939040
H	-3.0691643	4.3780217	-1.8537794
C	-2.9866090	3.3800918	-3.7800951

C	-2.4959525	2.2342671	-4.4782851
C	-1.7090730	1.2414821	-3.8073602
C	-3.7555356	4.3469749	-4.4581400
H	-4.1174446	5.2129420	-3.9018206
C	-4.0540289	4.2094340	-5.8109558
H	-4.6493786	4.9643814	-6.3224731
C	-3.5847736	3.0945554	-6.5059268
H	-3.8140055	2.9750235	-7.5658829
C	-2.8138330	2.1067225	-5.8670160
C	-2.3394820	0.9638060	-6.5811985
H	-2.5867665	0.8704853	-7.6402960
C	-1.5945662	0.0026093	-5.9621309
H	-1.2278361	-0.8728561	-6.4965887
C	-1.2454830	0.0976928	-4.5699980
O	-0.2249274	-3.7059201	-1.9687358
O	-0.8140270	-1.8230993	-0.0354414
O	-0.6892256	0.5833097	-1.7032980
O	-0.5292908	-0.8457521	-4.0692090
C	3.0400253	-0.2076094	-0.2974579
C	3.4496255	0.4465736	0.9112073
H	2.6777652	0.6746447	1.6492668
C	4.7586787	0.7640892	1.1510324
H	5.0359972	1.2684397	2.0785338
C	5.7822669	0.4480198	0.2120220
C	5.4173731	-0.2336574	-0.9893831
C	4.0526471	-0.5805030	-1.2551695
C	7.1299613	0.7820408	0.4539935
H	7.3834778	1.2994216	1.3804928
C	8.1263176	0.4617512	-0.4639575
H	9.1635256	0.7274055	-0.2647886
C	7.7853532	-0.2050244	-1.6412143
H	8.5582899	-0.4618489	-2.3671357
C	6.4533826	-0.5607488	-1.9193702
C	6.1072440	-1.2479628	-3.1235638
H	6.9015624	-1.4927525	-3.8311755
C	4.8162257	-1.6000069	-3.3916621
H	4.5433801	-2.1323250	-4.3020274
C	3.7466894	-1.2990221	-2.4779527
C	0.2149893	1.2835123	3.7800846
C	1.0302925	1.1471976	4.9608865
H	1.8987380	0.4937231	4.8796260
C	0.7326243	1.7964960	6.1242065
H	1.3704727	1.6730648	7.0017593
C	-0.4114836	2.6460528	6.2275513
C	-1.2529352	2.8058494	5.0815263
C	-0.9579837	2.1349344	3.8515488
C	-0.7184759	3.3165417	7.4258889
H	-0.0616016	3.1791734	8.2863147
C	-1.8369755	4.1428351	7.5251976
H	-2.0601133	4.6549169	8.4602055
C	-2.6677203	4.3076492	6.4179046
H	-3.5464435	4.9511857	6.4840772
C	-2.3976639	3.6557315	5.2004665
C	-3.2488998	3.8207722	4.0650712

H	-4.1238692	4.4670071	4.1597609
C	-2.9857534	3.1881404	2.8842661
H	-3.6362279	3.3065122	2.0179251
C	-1.8423645	2.3269386	2.7175041
O	1.7617235	-0.4276099	-0.4694500
O	2.5644585	-1.6979614	-2.7879995
O	0.5700986	0.6396337	2.7226110
O	-1.6675699	1.7692111	1.5690941

[Eu(PLN)₄Ca]⁺, motif 3, RI-B-P/def2-TZVPP
Energy = -3990.056968308

H	-7.0633712	1.7154670	4.6016937
H	-7.4114266	0.4751634	2.4716007
C	-6.2229164	1.5254936	3.9355536
C	-6.4159902	0.8302014	2.7429623
H	-6.5349468	-0.4848285	0.3909653
H	-4.7851919	2.5194055	5.2023359
C	-4.9465132	1.9757745	4.2701125
C	-5.3429211	0.5709621	1.8691551
C	-5.5307043	-0.1398035	0.6447839
C	-3.8465142	1.7426776	3.4233449
C	-4.0297021	1.0279857	2.1992677
C	-4.4865292	-0.3926851	-0.2001090
H	-4.6264791	-0.9398690	-1.1317487
H	-2.3958371	2.7396113	4.6970964
C	-2.5352672	2.2002274	3.7581445
C	-2.9253473	0.7755134	1.3269276
C	-3.1474040	0.0338410	0.1069363
C	-1.4696759	1.9757174	2.9326267
C	-1.6158339	1.2719866	1.6864554
H	2.8802008	-3.9681813	-7.8199779
H	2.6492674	-1.5144277	-7.4906611
O	-2.2077575	-0.2740658	-0.7236926
H	2.3195037	-6.2445693	-7.1682218
C	2.2828563	-3.5713813	-6.9968451
H	-2.9099112	6.9515683	-4.8263424
C	2.1659173	-2.2242716	-6.8201872
H	-2.6331701	4.6788455	-5.7964569
C	1.7210783	-5.8808860	-6.3314681
H	-2.3912215	8.5826385	-3.0971638
C	1.6195061	-4.4942862	-6.1287441
C	-2.3043794	6.1994371	-4.3169846
H	-0.4686750	2.3243056	3.1842457
C	-2.1622501	4.9537270	-4.8532132
H	1.1608555	-7.8591113	-5.6659583
C	1.3635246	-1.6628944	-5.7641927
C	1.0743747	-6.7880750	-5.4887261
C	-1.7850702	7.8521695	-2.5590833
O	1.2178127	-0.3894851	-5.7312740
C	-1.6573321	6.5589428	-3.0933520
O	-1.1804024	2.8357699	-4.8480996
C	0.8503329	-3.9844660	-5.0369577
C	-1.3486419	3.9443734	-4.2261146
C	0.7353890	-2.5712455	-4.8102340

H	-1.2613357	9.2204347	-0.9704680
C	-1.1545032	8.2111833	-1.3654424
C	0.3219168	-6.3098141	-4.4230876
C	-0.8773538	5.5751354	-2.4097076
O	-0.5702161	1.1223561	0.9464564
Ca	0.0310067	1.0292004	-4.5445279
C	0.2036087	-4.9242098	-4.1770334
C	-0.7357529	4.2468499	-2.9368068
H	-0.1899872	-7.0048339	-3.7557803
C	-0.3917770	7.2676710	-0.6882561
C	0.0111869	-2.1197858	-3.6512770
C	-0.2470738	5.9536143	-1.1848385
O	-0.0766250	-0.8535765	-3.2851832
C	-0.5577135	-4.4310397	-3.0819116
H	0.1078596	7.5317607	0.2450308
C	-0.0009840	3.2781058	-2.1660668
C	-0.6448092	-3.0877903	-2.8287314
O	0.1113400	2.0046263	-2.4981050
C	0.5251974	4.9826308	-0.4900071
H	-1.0723156	-5.1433311	-2.4346925
C	0.6380590	3.7008059	-0.9589535
H	-1.2295565	-2.7186136	-1.9858889
H	1.0273153	5.2720279	0.4347568
H	1.2297185	2.9626268	-0.4174657
Eu	0.0528803	0.0367472	-0.9557232
O	2.3253568	0.2260120	-0.7054905
H	4.7222789	1.0649796	-0.7989839
O	0.7627247	-1.8644502	0.0741114
C	3.3002017	-0.4418133	-0.1847875
C	4.6239510	0.1138973	-0.2767459
C	1.8406343	-2.3510160	0.5886508
C	3.1325046	-1.7094921	0.4880827
C	5.7038967	-0.5108581	0.2812791
H	6.6953095	-0.0598316	0.2061188
H	0.7626597	-4.0539384	1.3662416
C	1.7507706	-3.6007047	1.2954994
C	4.2741481	-2.3476709	1.0656883
C	5.5706494	-1.7537967	0.9718936
C	2.8516946	-4.1920223	1.8484118
C	4.1458044	-3.5946537	1.7522103
C	6.6808032	-2.3984642	1.5499065
H	7.6625427	-1.9297970	1.4655376
H	2.7545453	-5.1416045	2.3783727
C	5.2817397	-4.2026008	2.3191456
C	6.5410769	-3.6125139	2.2204171
H	5.1623060	-5.1522981	2.8429914
H	7.4097800	-4.0969169	2.6641600

[Eu(PLN)₄Ca]⁺, motif 4, RI-B-P/def2-TZVPP

Energy = -3990.050512115

H	7.4042724	-1.9573314	1.9113840
H	8.9094185	-1.9544046	-0.0710330
H	5.1805869	-1.6664983	2.9052511
C	7.0059693	-1.7305097	0.9212204

C	7.8504897	-1.7279517	-0.1881858
C	4.7617555	-1.4375286	1.9233589
C	5.6346494	-1.4428210	0.7921824
C	7.3318535	-1.4324684	-1.4490192
H	7.9862770	-1.4284526	-2.3220717
H	2.7613823	-1.1533771	2.6537751
C	3.4315292	-1.1545492	1.7948606
C	5.0892623	-1.1380386	-0.4946723
C	5.9685326	-1.1349156	-1.6234155
H	-0.5460473	-6.0951570	-3.9686015
H	-0.1392353	-3.6498528	-4.1523827
C	2.8418439	-0.8650310	0.5138097
C	3.7010495	-0.8435131	-0.6490440
C	5.4283296	-0.8309884	-2.9122472
H	6.1019085	-0.8323862	-3.7714981
C	-0.7624073	-5.4313955	-3.1291094
C	-0.5393095	-4.0911033	-3.2402521
H	-1.2585520	-8.0283406	-2.6601484
O	1.5735182	-0.6410721	0.4666222
C	3.1877510	-0.5217000	-1.9668198
C	4.1046784	-0.5432266	-3.0799333
C	-1.4925901	-7.3888953	-1.8075051
C	-1.2722985	-6.0065685	-1.9210543
C	-0.7793950	-3.1867935	-2.1406869
O	-0.4662603	-1.9589022	-2.2897216
H	0.0569313	8.1546914	3.3258639
H	-1.1510189	6.2447902	4.3711299
O	1.9641532	-0.2137697	-2.1936716
H	3.6897945	-0.3049543	-4.0586762
C	-0.0234129	7.2029503	2.8026690
C	-0.6965252	6.1357412	3.3852687
H	-1.9499859	3.9260476	4.2920664
H	1.0679581	7.8819576	1.0665832
C	0.5455574	7.0468762	1.5359763
C	-0.8107767	4.8962596	2.7188515
C	-1.5100833	3.8023140	3.3008477
C	0.4594468	5.8291607	0.8409593
C	-1.6320602	2.6097038	2.6379150
C	-0.2212046	4.7185858	1.4296078
H	-2.1499857	1.7682065	3.1019638
H	-2.1646360	-9.0249085	-0.5653263
C	-2.0042947	-7.9499122	-0.6340239
H	1.5443712	6.5290712	-0.9082977
C	1.0330856	5.6742691	-0.4612105
C	-1.0574868	2.3947273	1.3420317
C	-0.3172929	3.4668027	0.7390095
C	-1.5730189	-5.1435309	-0.8220619
C	-1.3504568	-3.7308634	-0.9152455
O	-1.2552639	1.2286262	0.7763323
C	0.9571379	4.4917390	-1.1360438
C	0.3126542	3.3339601	-0.5661261
Eu	-0.0188621	-0.0378502	-1.0460205
H	1.4006782	4.3646424	-2.1228324
O	0.3364382	2.2412834	-1.2270409

C	-2.3128215	-7.1236650	0.4395765
C	-2.1128639	-5.7275768	0.3649755
C	-1.7326102	-2.8948005	0.1863043
O	-2.4508189	0.4917891	-1.8343163
O	-1.6388785	-1.5853341	0.1782530
H	-1.1943519	0.7649886	-4.0324800
Ca	-3.1482146	0.0893680	0.2586619
H	-2.7202992	-7.5462972	1.3592488
C	-3.0628023	0.8099291	-2.9400121
C	-2.2651654	0.9465246	-4.1246650
C	-2.4439419	-4.8713891	1.4519782
C	-2.2688433	-3.5153742	1.3611473
O	-5.0091656	0.5877531	-0.7203674
H	-2.8434935	-5.3127434	2.3668604
H	-2.5098688	-2.8646131	2.2033393
C	-2.8081270	1.2856099	-5.3319974
H	-2.1694979	1.3798798	-6.2121620
C	-4.4883418	1.0345180	-3.0403123
C	-5.3909117	0.9143451	-1.9081512
C	-4.2060870	1.5226815	-5.4710277
C	-5.0388738	1.3943582	-4.3170615
H	-7.4348996	1.0720234	-1.2392377
C	-6.7910081	1.1695558	-2.1127933
H	-4.1058772	1.9655645	-7.5793172
C	-4.7662248	1.8758429	-6.7153397
C	-6.4391371	1.6359873	-4.4745935
C	-7.2910641	1.5134981	-3.3352802
H	-8.3594610	1.7000937	-3.4597731
C	-6.1317948	2.1079754	-6.8510609
C	-6.9581768	1.9877261	-5.7344358
H	-6.5508851	2.3805967	-7.8185669
H	-8.0305960	2.1670404	-5.8258551

[Eu(PLN)₄Sr]⁺, motif 1, RI-B-P/def2-TZVPP
Energy = -3343.155299778

Eu	0.1586721	-0.3810910	0.0477923
Sr	0.5580912	3.0655070	-0.6365522
C	-0.3176615	-3.3871950	-1.3637238
C	0.1498125	-4.2831284	-2.3867856
H	0.9038621	-3.8958178	-3.0708588
C	-0.3365063	-5.5553428	-2.5001074
H	0.0348244	-6.2135591	-3.2879715
C	-1.3326500	-6.0556102	-1.6067071
C	-1.8172081	-5.1973008	-0.5721323
C	-1.3131520	-3.8664310	-0.4295788
C	-1.8379425	-7.3641371	-1.7249566
H	-1.4527249	-8.0056463	-2.5190460
C	-2.8129860	-7.8432158	-0.8508067
H	-3.1937099	-8.8580010	-0.9573806
C	-3.2976903	-7.0144858	0.1592951
H	-4.0629570	-7.3790288	0.8462827
C	-2.8168059	-5.6999557	0.3162664
C	-3.3097239	-4.8415083	1.3446868
H	-4.0781429	-5.2234623	2.0195261

C	-2.8391794	-3.5664434	1.4964711
H	-3.2129607	-2.9120125	2.2829446
C	-1.8176971	-3.0347825	0.6378874
C	-1.5590950	3.4844444	-3.3135654
C	-2.0058458	4.4712502	-4.2671528
H	-1.5153657	5.4430206	-4.2185481
C	-2.9893556	4.2099727	-5.1723305
H	-3.3087936	4.9793359	-5.8780531
C	-3.6283273	2.9316267	-5.2211366
C	-3.2155122	1.9161424	-4.3015959
C	-2.1785887	2.1632159	-3.3374571
C	-4.6451078	2.6697097	-6.1546763
H	-4.9384714	3.4638662	-6.8430652
C	-5.2764850	1.4257772	-6.2133492
H	-6.0630177	1.2423898	-6.9439790
C	-4.8886586	0.4259977	-5.3291937
H	-5.3699539	-0.5527478	-5.3601248
C	-3.8712995	0.6485032	-4.3774723
C	-3.4727255	-0.3754955	-3.4740002
H	-3.9710186	-1.3453134	-3.5242174
C	-2.4834854	-0.1594151	-2.5560719
H	-2.1867867	-0.9577467	-1.8754169
C	-1.7966856	1.0955231	-2.4431290
O	0.1665263	-2.1915994	-1.3362425
O	-1.3952910	-1.8320682	0.8638500
O	-0.6415888	3.8250371	-2.4913138
O	-0.8621138	1.1929776	-1.5299776
C	3.3118175	-0.9495264	1.1064947
C	4.0888052	-1.7740443	1.9937671
H	3.5324590	-2.4330587	2.6592097
C	5.4534112	-1.7455309	1.9875106
H	6.0182636	-2.3915591	2.6623097
C	6.1761010	-0.8846612	1.1039326
C	5.4429716	-0.0311114	0.2228251
C	4.0098227	-0.0403259	0.2152205
C	7.5819179	-0.8613658	1.0950535
H	8.1206435	-1.5198247	1.7782341
C	8.2887240	-0.0171237	0.2365840
H	9.3776977	-0.0153145	0.2431266
C	7.5898626	0.8227670	-0.6237701
H	8.1289724	1.4899419	-1.2979954
C	6.1788814	0.8342503	-0.6433649
C	5.4563058	1.6957853	-1.5160551
H	6.0128460	2.3457413	-2.1936313
C	4.0868634	1.7130419	-1.5182086
H	3.5430055	2.3568842	-2.2117456
C	3.3130141	0.8675503	-0.6563836
C	0.4687474	4.2400993	2.6141145
C	0.7933267	5.3938595	3.4195074
H	1.2613250	6.2283103	2.8980455
C	0.5159419	5.4470943	4.7518257
H	0.7648436	6.3379124	5.3319165
C	-0.1098762	4.3494752	5.4231389
C	-0.4364022	3.1754969	4.6730650

C	-0.1468584	3.0888354	3.2698026
C	-0.3983644	4.4123541	6.7960193
H	-0.1360761	5.3187568	7.3439464
C	-1.0084179	3.3460031	7.4611990
H	-1.2263452	3.4156356	8.5259760
C	-1.3334649	2.1974958	6.7496413
H	-1.8110325	1.3554329	7.2529354
C	-1.0567029	2.0920184	5.3699328
C	-1.3898354	0.9176064	4.6395173
H	-1.8747524	0.0921558	5.1638486
C	-1.1153492	0.8151023	3.3034997
H	-1.3915266	-0.0868738	2.7536146
C	-0.4776654	1.8714208	2.5711955
O	2.0333899	-1.0651430	1.1396408
O	2.0101612	0.9804724	-0.7070279
O	0.7295249	4.2888774	1.3657143
O	-0.2354948	1.6633307	1.2994911

[Eu(PLN)₄Sr]⁺, motif 2, RI-B-P/def2-TZVPP

Energy = -3343.158398243

Eu	0.3856808	-1.5514396	-2.1326704
Sr	-0.3510184	0.3052200	0.8378488
C	-0.6516341	-4.6659607	-1.3279947
C	-0.5627418	-6.0341934	-1.7651032
H	0.0097527	-6.2182277	-2.6733733
C	-1.1755216	-7.0451533	-1.0840410
H	-1.0976509	-8.0738132	-1.4409918
C	-1.9327770	-6.7896519	0.1013008
C	-2.0362025	-5.4453858	0.5773985
C	-1.3935002	-4.3675994	-0.1159309
C	-2.5679287	-7.8325258	0.7980755
H	-2.4723966	-8.8504059	0.4169947
C	-3.3098846	-7.5869178	1.9547793
H	-3.7959209	-8.4082118	2.4793573
C	-3.4230112	-6.2845252	2.4297246
H	-4.0015911	-6.0768416	3.3310562
C	-2.7979596	-5.2101593	1.7630384
C	-2.9134185	-3.8744054	2.2411349
H	-3.5048257	-3.6853497	3.1386571
C	-2.3001237	-2.8374676	1.5925377
H	-2.4154454	-1.8194378	1.9695990
C	-1.5067478	-3.0314388	0.4125473
C	-1.4905198	1.3633380	-2.4076607
C	-2.0070557	2.5288895	-1.7483277
H	-1.7790279	2.6622116	-0.6888304
C	-2.7806068	3.4485313	-2.4018736
H	-3.1563321	4.3230357	-1.8675930
C	-3.1146756	3.2910168	-3.7773325
C	-2.6277737	2.1393209	-4.4683159
C	-1.8145682	1.1657833	-3.8003081
C	-3.9103693	4.2386694	-4.4526113
H	-4.2682644	5.1099522	-3.9019975
C	-4.2392582	4.0752900	-5.7949744
H	-4.8549759	4.8149797	-6.3046602

C	-3.7738329	2.9538441	-6.4825761
H	-4.0269555	2.8142258	-7.5346461
C	-2.9767564	1.9853968	-5.8465486
C	-2.5057586	0.8357377	-6.5527094
H	-2.7764978	0.7222106	-7.6041083
C	-1.7351176	-0.1066077	-5.9363691
H	-1.3704535	-0.9860460	-6.4657140
C	-1.3537498	0.0148971	-4.5543895
O	-0.0754937	-3.7696164	-2.0445450
O	-0.9287502	-1.9835444	-0.1133831
O	-0.7527507	0.5427169	-1.7069571
O	-0.6139237	-0.9107137	-4.0559718
C	3.0052196	-0.3256840	-0.2057212
C	3.4075837	0.2275352	1.0553573
H	2.6346401	0.4051200	1.8068915
C	4.7154585	0.5210855	1.3313214
H	4.9860254	0.9459424	2.2996789
C	5.7449725	0.2824046	0.3766196
C	5.3867001	-0.2902262	-0.8821657
C	4.0232168	-0.6114821	-1.1855694
C	7.0921010	0.5908776	0.6559975
H	7.3401590	1.0243753	1.6260156
C	8.0933624	0.3506463	-0.2800560
H	9.1298407	0.5949665	-0.0519062
C	7.7581688	-0.2075301	-1.5144843
H	8.5351652	-0.3997464	-2.2559379
C	6.4276246	-0.5338974	-1.8315679
C	6.0869139	-1.1075359	-3.0956719
H	6.8850103	-1.2883392	-3.8181802
C	4.7971085	-1.4303330	-3.4027433
H	4.5290667	-1.8755837	-4.3600818
C	3.7219428	-1.2142518	-2.4710541
C	0.1880223	1.4652254	4.0269744
C	0.9905138	1.3157042	5.2169294
H	1.7844322	0.5701764	5.1747263
C	0.7691596	2.0589469	6.3390750
H	1.3936421	1.9205967	7.2239862
C	-0.2784694	3.0293620	6.3893776
C	-1.1030549	3.2117654	5.2329810
C	-0.8885353	2.4433451	4.0442377
C	-0.5065881	3.7949574	7.5469639
H	0.1357937	3.6364992	8.4146386
C	-1.5300416	4.7403815	7.5981988
H	-1.6933651	5.3248365	8.5026392
C	-2.3429194	4.9305838	6.4815430
H	-3.1475638	5.6670451	6.5095553
C	-2.1495553	4.1864863	5.3037744
C	-2.9845969	4.3806911	4.1607440
H	-3.7831526	5.1229987	4.2194040
C	-2.7979697	3.6586870	3.0185930
H	-3.4352871	3.7991823	2.1457946
C	-1.7568631	2.6668958	2.8988448
O	1.7284901	-0.5369031	-0.4002595
O	2.5418523	-1.5808625	-2.8234070

O	0.4670305	0.7219759	3.0162670
O	-1.6567002	2.0313822	1.7858845

[Eu(PLN)₄Sr]⁺, motif 3, RI-B-P/def2-TZVPP
 Energy = -3343.140188447

H	-7.1659362	1.7269621	4.3328439
H	-7.4732344	0.4946038	2.1917871
C	-6.3126945	1.5380031	3.6828501
C	-6.4829384	0.8473086	2.4842473
H	-6.5565684	-0.4601406	0.1262439
H	-4.8988158	2.5249681	4.9815943
C	-5.0423873	1.9849809	4.0443488
C	-5.3929727	0.5897107	1.6310263
C	-5.5572280	-0.1167147	0.4008381
C	-3.9261394	1.7532570	3.2189526
C	-4.0858385	1.0435531	1.9886272
C	-4.4967605	-0.3674608	-0.4240840
H	-4.6190970	-0.9118882	-1.3598672
H	-2.4998657	2.7431192	4.5254835
C	-2.6210702	2.2076437	3.5817601
C	-2.9646844	0.7930990	1.1372384
C	-3.1631491	0.0568987	-0.0899819
C	-1.5397156	1.9852084	2.7768031
C	-1.6616977	1.2865344	1.5247830
H	3.1199479	-4.1905312	-7.6335125
H	2.8469710	-1.7257351	-7.4562691
O	-2.2084850	-0.2481049	-0.9044086
H	2.5411528	-6.4324759	-6.8916485
C	2.4779682	-3.7555419	-6.8649817
H	-3.2463005	7.0648918	-4.2616681
C	2.3385933	-2.4029513	-6.7705237
H	-3.0417329	4.8687635	-5.4090326
C	1.8993768	-6.0312315	-6.1056868
H	-2.5482928	8.5986393	-2.5086492
C	1.7783785	-4.6373217	-5.9819094
C	-2.5696228	6.2981327	-3.8793330
H	-0.5435055	2.3318737	3.0491174
C	-2.4680207	5.0943059	-4.5105315
H	1.3195681	-7.9774398	-5.3657403
C	1.4729108	-1.7917540	-5.7924444
C	1.2177509	-6.8994370	-5.2491351
C	-1.8693459	7.8516954	-2.0942637
O	1.2930927	-0.5264301	-5.8522476
C	-1.7854648	6.5973240	-2.7207226
O	-1.4277591	3.0189384	-4.7746417
C	0.9537604	-4.0771166	-4.9568341
C	-1.5613466	4.0691106	-4.0562186
C	0.8178765	-2.6546531	-4.8115259
H	-1.1793565	9.1338101	-0.4969378
C	-1.1049168	8.1529026	-0.9642091
C	0.4113935	-6.3728990	-4.2479451
C	-0.9138567	5.5914916	-2.1980128
O	-0.6021231	1.1388589	0.8058595
Sr	-0.0759019	1.0870592	-4.8114671

C	0.2732737	-4.9774093	-4.0802837
C	-0.8159723	4.3011841	-2.8210375
H	-0.1283892	-7.0364625	-3.5706162
C	-0.2515945	7.1882503	-0.4434419
C	0.0467263	-2.1502812	-3.7052968
C	-0.1480151	5.9097013	-1.0343553
O	-0.0538505	-0.8700489	-3.3971642
C	-0.5419529	-4.4352665	-3.0490828
H	0.3530119	7.4069700	0.4380757
C	0.0078575	3.2999613	-2.1956389
C	-0.6444218	-3.0818464	-2.8676714
O	0.0836367	2.0454420	-2.6016600
C	0.7151383	4.9157928	-0.4966451
H	-1.0837994	-5.1176076	-2.3918383
C	0.7839846	3.6653165	-1.0505858
H	-1.2682448	-2.6733707	-2.0720613
H	1.3214399	5.1609012	0.3771339
H	1.4448910	2.9062079	-0.6307994
Eu	0.0607454	0.0649018	-1.0904408
O	2.3343452	0.2581611	-0.8231721
H	4.7372593	1.0787988	-0.9361175
O	0.7619516	-1.8139696	-0.0104008
C	3.3053790	-0.4054511	-0.2898805
C	4.6327813	0.1397814	-0.3935693
C	1.8354025	-2.2912525	0.5203501
C	3.1306906	-1.6581349	0.4085804
C	5.7092795	-0.4799910	0.1765260
H	6.7035698	-0.0372115	0.0908280
H	0.7467813	-3.9686849	1.3376002
C	1.7375917	-3.5229380	1.2577129
C	4.2683187	-2.2900081	1.0010574
C	5.5685663	-1.7066708	0.8941025
C	2.8343635	-4.1071678	1.8257775
C	4.1322540	-3.5201715	1.7159337
C	6.6748923	-2.3454526	1.4859613
H	7.6596203	-1.8852125	1.3905696
H	2.7312815	-5.0432084	2.3782602
C	5.2643215	-4.1221998	2.2965246
C	6.5275887	-3.5429670	2.1838565
H	5.1387960	-5.0587710	2.8421499
H	7.3932846	-4.0229352	2.6381884

[Eu(PLN)₄Sr]⁺, motif 4, RI-B-P/def2-TZVPP

Energy = -3343.137032028

H	7.4687849	-1.8234254	1.7096088
H	8.9433605	-1.3828799	-0.2467440
H	5.2398496	-1.8876438	2.7329941
C	7.0404688	-1.4789003	0.7670552
C	7.8674970	-1.2337732	-0.3282944
C	4.7912857	-1.5429439	1.7991862
C	5.6484055	-1.2905471	0.6841986
C	7.3090395	-0.7973851	-1.5297856
H	7.9494310	-0.6030788	-2.3915947
H	2.7835526	-1.5483831	2.5634313

C	3.4400188	-1.3613103	1.7143668
C	5.0621881	-0.8437943	-0.5416345
C	5.9225886	-0.6002519	-1.6585160
H	-0.4420220	-6.3199144	-3.7532782
H	0.0822546	-3.8946179	-3.9071785
C	2.8152619	-0.8922827	0.5046574
C	3.6523331	-0.6459699	-0.6483208
C	5.3416882	-0.1524410	-2.8862574
H	6.0018790	0.0354881	-3.7353342
C	-0.7100720	-5.6409213	-2.9413940
C	-0.4210436	-4.3118581	-3.0358036
H	-1.3624030	-8.2098716	-2.5138327
O	1.5392215	-0.7122670	0.5116609
C	3.0924124	-0.2087310	-1.9124403
C	3.9960179	0.0395413	-3.0091707
C	-1.6470762	-7.5549444	-1.6888046
C	-1.3582276	-6.1838136	-1.7862233
C	-0.7376450	-3.3892834	-1.9723909
O	-0.3795442	-2.1708444	-2.1011698
H	0.3231684	8.0189353	3.3018155
H	-0.5992793	6.0622865	4.5342905
O	1.8376735	-0.0358785	-2.1076768
H	3.5483518	0.3750775	-3.9439801
C	0.1755023	7.0680779	2.7917856
C	-0.3383284	5.9751800	3.4784450
H	-1.3267955	3.7183170	4.5776596
H	0.8891750	7.7963027	0.8868589
C	0.4959904	6.9398756	1.4369856
C	-0.5379998	4.7363410	2.8299985
C	-1.0808044	3.6160708	3.5190562
C	0.3206657	5.7244343	0.7564047
C	-1.2941797	2.4256525	2.8740885
C	-0.1967952	4.5869132	1.4504158
H	-1.6927866	1.5634400	3.4116402
H	-2.4993120	-9.1521459	-0.5087522
C	-2.2872985	-8.0854554	-0.5656851
H	1.0191621	6.4742895	-1.1615452
C	0.6366611	5.5976166	-0.6349213
C	-0.9701553	2.2410351	1.4896785
C	-0.3785349	3.3360430	0.7759752
C	-1.7219148	-5.3007549	-0.7223112
C	-1.4340199	-3.8994661	-0.8008218
O	-1.2567287	1.0813212	0.9459224
C	0.4785038	4.4162679	-1.2961473
C	0.0108684	3.2260593	-0.6244424
Eu	-0.1398802	-0.1777928	-0.9406926
H	0.7313393	4.3102498	-2.3504759
O	-0.0233241	2.1344578	-1.2816077
C	-2.6542491	-7.2397429	0.4743100
C	-2.3878111	-5.8545931	0.4143102
C	-1.8645652	-3.0373994	0.2649154
O	-2.5519322	0.3163261	-1.7381927
O	-1.7106959	-1.7376348	0.2694295
H	-1.1528750	0.3477719	-3.8718521

Sr	-3.3788751	0.0268825	0.4953482
H	-3.1587697	-7.6391141	1.3554450
C	-3.0612696	0.6553949	-2.8886781
C	-2.1888106	0.6490118	-4.0291971
C	-2.7693147	-4.9787550	1.4690019
C	-2.5229545	-3.6333111	1.3929427
O	-5.1506918	0.7315413	-0.7946570
H	-3.2606918	-5.3978438	2.3490338
H	-2.7907697	-2.9738206	2.2211677
C	-2.6176306	0.9986005	-5.2783102
H	-1.9229792	0.9811060	-6.1201154
C	-4.4434722	1.0347766	-3.0865108
C	-5.4199138	1.0592838	-2.0101217
C	-3.9672398	1.3904224	-5.5109827
C	-4.8737212	1.4041672	-4.4064495
H	-7.4679440	1.4777633	-1.4773168
C	-6.7667554	1.4675655	-2.3113593
H	-3.6937924	1.7339759	-7.6223281
C	-4.4090874	1.7558805	-6.7986169
C	-6.2247552	1.7986222	-4.6592967
C	-7.1506833	1.8198464	-3.5721685
H	-8.1806083	2.1234406	-3.7696277
C	-5.7275134	2.1385261	-7.0262733
C	-6.6251017	2.1583536	-5.9592236
H	-6.0553109	2.4192571	-8.0261782
H	-7.6619452	2.4566960	-6.1223002

#Ca Motif 1 BHLYP-D3

90

Energy = -3988.031569498

Eu	0.2390514	-0.5569152	0.2533797
C	-0.6332101	-3.2713437	-1.3992983
C	-0.4257369	-4.0213346	-2.5955317
H	0.3213043	-3.6521545	-3.2709192
C	-1.1331975	-5.1333630	-2.8585845
H	-0.9574408	-5.6806527	-3.7670795
C	-2.1205100	-5.6171672	-1.9585566
C	-2.3536056	-4.9030960	-0.7677260
C	-1.6203601	-3.7221118	-0.4713855
C	-2.8464432	-6.7690034	-2.2309319
H	-2.6522349	-7.3003562	-3.1445829
C	-3.8008342	-7.2355700	-1.3522331
H	-4.3524400	-8.1278303	-1.5757029
C	-4.0365727	-6.5461996	-0.1841743
H	-4.7764599	-6.9008522	0.5097323
C	-3.3295019	-5.3889329	0.1224470
C	-3.5648589	-4.6741960	1.3253407
H	-4.3098747	-5.0463938	2.0051007
C	-2.8812111	-3.5543636	1.6230203
H	-3.0592057	-3.0101150	2.5301327
C	-1.8887332	-3.0310956	0.7442711

C	-1.2303727	2.9269518	-3.2649535
C	-1.4128187	3.7570748	-4.4208885
H	-0.8657255	4.6797727	-4.4334552
C	-2.2352225	3.4080573	-5.4191566
H	-2.3589376	4.0553790	-6.2685722
C	-2.9715276	2.1892790	-5.3863026
C	-2.8115156	1.3310432	-4.2792741
C	-1.9287915	1.6662455	-3.2126528
C	-3.8288901	1.8449924	-6.4163381
H	-3.9313441	2.5147753	-7.2504066
C	-4.5494281	0.6649006	-6.3879330
H	-5.2114604	0.4157652	-7.1941494
C	-4.4078498	-0.1792346	-5.3163834
H	-4.9625365	-1.0986696	-5.2755608
C	-3.5491262	0.1328182	-4.2624028
C	-3.4049135	-0.7300694	-3.1526457
H	-3.9805503	-1.6373134	-3.1218677
C	-2.5643800	-0.4326273	-2.1436388
H	-2.4711513	-1.0908982	-1.3025725
C	-1.7762314	0.7505362	-2.1456538
O	0.0685419	-2.2324605	-1.2206064
O	-1.2952283	-1.9587885	1.0888800
O	-0.4853705	3.3486600	-2.3517015
O	-0.9561877	0.9189907	-1.1623373
C	3.4516175	-0.7959014	1.0735639
C	4.3609797	-1.5764428	1.8488583
H	3.9338377	-2.3554460	2.4497578
C	5.6847752	-1.3522963	1.8127257
H	6.3499005	-1.9596487	2.3994905
C	6.2434845	-0.3229445	1.0070338
C	5.3769345	0.4791869	0.2394081
C	3.9715649	0.2639966	0.2644490
C	7.6111878	-0.0982559	0.9715147
H	8.2540976	-0.7210234	1.5660848
C	8.1530530	0.9042450	0.1916075
H	9.2135313	1.0630769	0.1747841
C	7.3188623	1.6955331	-0.5601916
H	7.7257042	2.4802486	-1.1711292
C	5.9392178	1.5013989	-0.5470752
C	5.0734918	2.3135129	-1.3162844
H	5.4995749	3.0868471	-1.9291810
C	3.7385007	2.1292351	-1.2938182
H	3.0891959	2.7343785	-1.8997723
C	3.1352838	1.1156247	-0.4991469
C	0.3545941	4.0217577	2.6528826
C	0.6482260	5.2233050	3.3799027
H	0.9796055	6.0610079	2.7974464
C	0.5058014	5.2975101	4.7098841
H	0.7280726	6.2135730	5.2268565
C	0.0569056	4.1827679	5.4742246
C	-0.2345809	2.9763784	4.8054027
C	-0.0844826	2.8655106	3.3933629
C	-0.0920651	4.2714521	6.8471059
H	0.1377053	5.2016713	7.3336156

C	-0.5281980	3.1927266	7.5944264
H	-0.6394209	3.2805410	8.6575427
C	-0.8164564	2.0120974	6.9589088
H	-1.1576072	1.1637747	7.5233862
C	-0.6751765	1.8852380	5.5770097
C	-0.9734043	0.6717344	4.9174293
H	-1.3226376	-0.1611050	5.5003908
C	-0.8316676	0.5481981	3.5833323
H	-1.0834098	-0.3733494	3.0907660
C	-0.3700306	1.6250708	2.7758149
O	2.2243387	-1.0867009	1.1319947
O	1.8524509	1.0407932	-0.5113351
O	0.4873308	4.0420633	1.4084412
O	-0.2332092	1.3977000	1.5133544
Ca	0.2456137	2.7588256	-0.3609707

#Ca Motif 2, BHLYP-D3

90

Energy = -3988.034642492

Eu	0.1000194	-0.5067158	-2.0994605
C	0.3489720	-3.7958711	-1.7313129
C	0.4769827	-5.0021228	-2.4818322
H	0.5248830	-4.9018949	-3.5485666
C	0.5344824	-6.2003346	-1.8771853
H	0.6306747	-7.0955768	-2.4643829
C	0.4719698	-6.3231862	-0.4627661
C	0.3463406	-5.1539738	0.3117014
C	0.2797061	-3.8748566	-0.3058529
C	0.5329349	-7.5626959	0.1565108
H	0.6282084	-8.4423317	-0.4532386
C	0.4737448	-7.6805891	1.5305928
H	0.5222478	-8.6468981	1.9932331
C	0.3533255	-6.5468821	2.2979004
H	0.3075301	-6.6227666	3.3687279
C	0.2885609	-5.2856675	1.7107309
C	0.1678801	-4.1127982	2.4926649
H	0.1286582	-4.2065664	3.5626080
C	0.1036241	-2.8939966	1.9227343
H	0.0184118	-2.0159663	2.5363337
C	0.1495025	-2.7244367	0.5111007
C	-2.6403083	1.2166946	-1.0195011
C	-3.2979684	1.8217484	0.0872128
H	-2.8154751	1.7801566	1.0459131
C	-4.5019573	2.4118448	-0.0447517
H	-4.9718324	2.8631884	0.8102494
C	-5.1751387	2.4512705	-1.2882967
C	-4.5645450	1.8399840	-2.3976316
C	-3.2952503	1.2087735	-2.2778359
C	-6.4166214	3.0673144	-1.4239716
H	-6.8635036	3.5267409	-0.5615209
C	-7.0674851	3.0930531	-2.6342277
H	-8.0227171	3.5716061	-2.7274871
C	-6.4787384	2.4937778	-3.7292592
H	-6.9784587	2.5059800	-4.6804599
C	-5.2441524	1.8692003	-3.6306496

C	-4.6407614	1.2474920	-4.7566938
H	-5.1629033	1.2723330	-5.6959827
C	-3.4484378	0.6356102	-4.6650264
H	-2.9881216	0.1595415	-5.5086858
C	-2.7311259	0.5853669	-3.4332296
O	0.3047122	-2.7052150	-2.3688927
O	0.0682484	-1.5265930	0.0527549
O	-1.4747645	0.7095476	-0.8134060
O	-1.6212143	-0.0200507	-3.4222126
C	2.5045533	1.5315613	-0.7903088
C	3.0252001	2.1400953	0.3852723
H	2.5048349	1.9757794	1.3105824
C	4.1525444	2.8774995	0.3574969
H	4.5197699	3.3264964	1.2624887
C	4.8771852	3.0761368	-0.8412443
C	4.4058703	2.4637063	-2.0160413
C	3.2224827	1.6746929	-2.0049065
C	6.0362423	3.8474676	-0.8711346
H	6.3782100	4.3036992	0.0396340
C	6.7378963	4.0285679	-2.0389552
H	7.6283973	4.6261143	-2.0506387
C	6.2851219	3.4308218	-3.1977324
H	6.8260304	3.5643154	-4.1165595
C	5.1369428	2.6525943	-3.2046425
C	4.6738371	2.0318540	-4.3959551
H	5.2342066	2.1801821	-5.3012386
C	3.5670138	1.2706404	-4.4062588
H	3.2148538	0.7927522	-5.2995064
C	2.8036590	1.0526298	-3.2212198
C	1.0499371	0.9304545	4.1429717
C	2.2245004	0.9579541	4.9625810
H	3.1630533	0.8391784	4.4559226
C	2.1564481	1.1179271	6.2937835
H	3.0559651	1.1332129	6.8826820
C	0.9104501	1.2696363	6.9595940
C	-0.2698091	1.2480144	6.1908085
C	-0.2216004	1.0781900	4.7791963
C	0.8439522	1.4365599	8.3366286
H	1.7583688	1.4497606	8.9011581
C	-0.3651029	1.5848144	8.9798876
H	-0.4014243	1.7135769	10.0441169
C	-1.5268312	1.5662398	8.2399065
H	-2.4771745	1.6816385	8.7283415
C	-1.4991606	1.4009874	6.8614276
C	-2.6958848	1.3816603	6.0959204
H	-3.6333269	1.4965889	6.6098633
C	-2.6724764	1.2233627	4.7630603
H	-3.5746871	1.2040862	4.1823327
C	-1.4455530	1.0662329	4.0407401
O	1.3968539	0.8844557	-0.6838439
O	1.7869026	0.3056996	-3.3035768
O	1.2038516	0.7743373	2.8989553
O	-1.5145702	0.9231710	2.7872095
Ca	-0.1010800	0.5452234	1.1409679

#Mg Motif 1, BHLYP-D3

90

Energy = -3510.502551794

Eu	0.3613626	-0.3648982	0.7127580
C	1.2664505	-3.4909417	1.1743877
C	2.0850946	-4.5491212	0.6812250
H	2.7192436	-4.3183991	-0.1525449
C	2.0610289	-5.7728390	1.2383136
H	2.6891067	-6.5536997	0.8490090
C	1.2202755	-6.0694976	2.3433516
C	0.3972937	-5.0489527	2.8561213
C	0.4043354	-3.7495102	2.2807246
C	1.1999546	-7.3336312	2.9189996
H	1.8369130	-8.0982081	2.5134351
C	0.3836512	-7.6152556	3.9928390
H	0.3793482	-8.5957318	4.4274856
C	-0.4249324	-6.6242937	4.5033911
H	-1.0647507	-6.8310953	5.3415730
C	-0.4313366	-5.3476370	3.9537889
C	-1.2593806	-4.3209918	4.4765567
H	-1.8912410	-4.5497854	5.3156057
C	-1.2657364	-3.0845416	3.9465522
H	-1.8910274	-2.3067210	4.3397304
C	-0.4429541	-2.7464379	2.8337517
C	-1.0150922	-0.1820269	-4.1530842
C	-1.0732095	-0.0625068	-5.5802229
H	-1.0708639	0.9350386	-5.9745025
C	-1.1432794	-1.1397955	-6.3745810
H	-1.1936309	-1.0202008	-7.4417890
C	-1.1614120	-2.4614548	-5.8422220
C	-1.0917941	-2.6274966	-4.4447325
C	-1.0029263	-1.5024798	-3.5796845
C	-1.2442313	-3.5679481	-6.6683310
H	-1.2943120	-3.4192299	-7.7314018
C	-1.2645166	-4.8509520	-6.1504852
H	-1.3315996	-5.6968533	-6.8064401
C	-1.1991785	-5.0275801	-4.7921501
H	-1.2161125	-6.0175502	-4.3746558
C	-1.1105870	-3.9353362	-3.9280793
C	-1.0447230	-4.1059727	-2.5267444
H	-1.0736825	-5.1023650	-2.1247665
C	-0.9480529	-3.0484720	-1.6962123
H	-0.9009799	-3.1864907	-0.6342577
C	-0.9057250	-1.7194774	-2.1898707
O	1.3395820	-2.3651790	0.5940762
O	-0.5108072	-1.5567560	2.3855165
O	-0.9908750	0.8731839	-3.4780884
O	-0.7815061	-0.7609268	-1.3297116
C	2.8659530	1.7631142	1.2012983
C	3.8758884	2.0920303	2.1520546
H	3.8790786	1.5289819	3.0649274
C	4.7803731	3.0564331	1.9096382
H	5.5350470	3.2823263	2.6410735
C	4.7681567	3.7992082	0.6991288

C	3.7817129	3.5062345	-0.2614210
C	2.8216875	2.4833416	-0.0313599
C	5.6986249	4.7997789	0.4561705
H	6.4438338	5.0069198	1.2020999
C	5.6782118	5.5250434	-0.7172045
H	6.4044646	6.2950066	-0.8901507
C	4.7156684	5.2518914	-1.6607122
H	4.6861653	5.8114281	-2.5775736
C	3.7663513	4.2554259	-1.4519139
C	2.7681529	3.9726333	-2.4156634
H	2.7541893	4.5444034	-3.3256687
C	1.8487112	3.0092611	-2.2131999
H	1.0983381	2.7945877	-2.9507272
C	1.8429344	2.2305526	-1.0246754
C	-2.3060240	3.6872587	-0.6304770
C	-2.7677759	4.9987006	-0.9796050
H	-2.5973482	5.3090072	-1.9921212
C	-3.3842394	5.7881996	-0.0888349
H	-3.7231436	6.7662029	-0.3794662
C	-3.6113283	5.3672698	1.2536715
C	-3.1715054	4.0865194	1.6426547
C	-2.5152266	3.2295482	0.7179295
C	-4.2472936	6.1881149	2.1677203
H	-4.5753265	7.1612036	1.8510669
C	-4.4653296	5.7783528	3.4713590
H	-4.9612239	6.4282292	4.1656548
C	-4.0411261	4.5348935	3.8642952
H	-4.2031660	4.2026925	4.8732454
C	-3.3951570	3.6796228	2.9704536
C	-2.9545918	2.3960657	3.3650519
H	-3.1291970	2.0792696	4.3772209
C	-2.3308003	1.5714253	2.4985515
H	-2.0132049	0.5892322	2.7972544
C	-2.0858838	1.9604106	1.1557090
O	2.0512020	0.8402250	1.5013773
O	0.9391466	1.3264133	-0.9082489
O	-1.7471563	3.0062791	-1.5209285
O	-1.4680629	1.1183690	0.3943153
Mg	-0.9709921	1.2516293	-1.5957544

#Mg Motif 2, BHLYP-D3

90

Energy = -3510.502430760

Eu	-0.0183253	-1.2464820	-1.7095201
C	-0.7281899	-3.9757255	0.0468909
C	-0.8515638	-5.3917407	-0.0722633
H	-0.6766429	-5.8091123	-1.0446293
C	-1.1751999	-6.1585063	0.9824421
H	-1.2638480	-7.2235361	0.8668297
C	-1.4118070	-5.5954341	2.2654613
C	-1.2949462	-4.2010851	2.4232066
C	-0.9431871	-3.3692967	1.3245905
C	-1.7526859	-6.3909489	3.3490337
H	-1.8350556	-7.4528326	3.2067413
C	-1.9863064	-5.8426535	4.5943580

H	-2.2502502	-6.4719694	5.4216998
C	-1.8784447	-4.4829380	4.7607409
H	-2.0594340	-4.0412801	5.7234210
C	-1.5355334	-3.6530535	3.6957289
C	-1.4265582	-2.2521953	3.8565338
H	-1.6184557	-1.8261233	4.8244307
C	-1.0895749	-1.4505213	2.8274364
H	-1.0137222	-0.3910692	2.9661166
C	-0.8238419	-1.9739329	1.5350198
C	-2.0067564	1.5314163	-1.7400678
C	-2.3922254	2.7341930	-1.0864976
H	-1.9638751	2.9265598	-0.1240371
C	-3.2810781	3.5826273	-1.6364720
H	-3.5499993	4.4843155	-1.1164652
C	-3.8837011	3.3190864	-2.8893101
C	-3.5335926	2.1348501	-3.5613530
C	-2.5908044	1.2261545	-3.0016505
C	-4.8044812	4.1981326	-3.4508801
H	-5.0545366	5.0963267	-2.9166991
C	-5.3905064	3.9326348	-4.6666209
H	-6.0987491	4.6178508	-5.0898035
C	-5.0567759	2.7740351	-5.3351271
H	-5.5076445	2.5533152	-6.2851803
C	-4.1420135	1.8743126	-4.8043859
C	-3.8018832	0.6815603	-5.4937425
H	-4.2703497	0.4845749	-6.4409159
C	-2.9141379	-0.1901428	-4.9860828
H	-2.6481764	-1.0934255	-5.4994719
C	-2.2738505	0.0454487	-3.7358668
O	-0.4374805	-3.3194560	-0.9939141
O	-0.4880531	-1.1454685	0.6070725
O	-1.1419715	0.7827279	-1.1530993
O	-1.4385184	-0.8211452	-3.3349826
C	2.6323149	0.7694333	-0.9467726
C	3.1040119	1.8704248	-0.1831263
H	2.4367189	2.2983846	0.5363767
C	4.3557366	2.3458951	-0.3262103
H	4.6821155	3.1790079	0.2693462
C	5.2649670	1.7704062	-1.2441574
C	4.8299674	0.6826977	-2.0214322
C	3.5082032	0.1721314	-1.8902133
C	6.5613448	2.2587005	-1.3859800
H	6.8694723	3.0918038	-0.7813460
C	7.4391890	1.6927991	-2.2793634
H	8.4356070	2.0765689	-2.3796554
C	7.0233222	0.6245814	-3.0476604
H	7.6999763	0.1732498	-3.7498445
C	5.7387100	0.1132885	-2.9342593
C	5.3112237	-0.9843329	-3.7276429
H	6.0090159	-1.4179951	-4.4208168
C	4.0654829	-1.4773018	-3.6284209
H	3.7319935	-2.3021132	-4.2273473
C	3.1163591	-0.9223465	-2.7209312
C	1.1538819	1.3818792	3.2723690

C	2.2295429	1.1514372	4.1901746
H	3.0565809	0.5742211	3.8240045
C	2.1970034	1.6277193	5.4451882
H	3.0160081	1.4365583	6.1151527
C	1.0961274	2.3908770	5.9264272
C	0.0216719	2.6442045	5.0522919
C	0.0331759	2.1446638	3.7227693
C	1.0663215	2.8857232	7.2223038
H	1.8957359	2.6825669	7.8748308
C	-0.0029492	3.6284328	7.6782046
H	-0.0111067	4.0047641	8.6826108
C	-1.0571373	3.8852533	6.8310094
H	-1.8940002	4.4656006	7.1741772
C	-1.0624427	3.4062653	5.5259298
C	-2.1422689	3.6679744	4.6408338
H	-2.9706306	4.2498571	5.0030726
C	-2.1452424	3.2064817	3.3780784
H	-2.9630096	3.3988671	2.7105063
C	-1.0645920	2.4252704	2.8630388
O	1.4227239	0.3747904	-0.7500086
O	1.9575604	-1.4305710	-2.7000405
O	1.2459009	0.8978213	2.1132979
O	-1.1454257	2.0152934	1.6650145
Mg	-0.0267742	0.8255952	0.6417535

#Sr Motif 1, BHLYP-D3

90

Energy = -3341.080812418

Eu	0.2293120	0.6759899	0.1800603
C	1.2385474	1.9184730	3.0637443
C	2.2935904	1.9144808	4.0249090
H	3.1581109	1.3257593	3.7872274
C	2.2046147	2.6149471	5.1682372
H	3.0140899	2.5957304	5.8754541
C	1.0574099	3.3949332	5.4756848
C	-0.0049053	3.4220304	4.5521068
C	0.0654105	2.6843240	3.3396437
C	0.9708875	4.1223621	6.6550282
H	1.7932220	4.0895891	7.3460408
C	-0.1438590	4.8797202	6.9461954
H	-0.1952307	5.4375920	7.8608014
C	-1.1885215	4.9145182	6.0503746
H	-2.0618576	5.5027365	6.2648738
C	-1.1374643	4.1992518	4.8590607
C	-2.2089072	4.2317454	3.9295292
H	-3.0731686	4.8263685	4.1643854
C	-2.1609062	3.5390492	2.7772992
H	-2.9709384	3.5576489	2.0742441
C	-1.0326089	2.7380851	2.4358112
C	0.0198874	-4.3147692	1.6445063
C	0.2611618	-5.6398543	2.1428925
H	0.4813359	-6.3895924	1.4077685
C	0.1954424	-5.9277774	3.4487679
H	0.3716578	-6.9316054	3.7910437
C	-0.1169789	-4.9298191	4.4161010

C	-0.3418041	-3.6083679	3.9782290
C	-0.2533282	-3.2666505	2.5976189
C	-0.1992977	-5.2424910	5.7611602
H	-0.0196270	-6.2563746	6.0686146
C	-0.5077718	-4.2805767	6.7058309
H	-0.5701852	-4.5419907	7.7441611
C	-0.7344500	-2.9917177	6.2966917
H	-0.9794898	-2.2312851	7.0153188
C	-0.6538766	-2.6392395	4.9494678
C	-0.8935957	-1.3142461	4.5225390
H	-1.1559018	-0.5713694	5.2538249
C	-0.7979498	-0.9740960	3.2238509
H	-0.9945027	0.0329309	2.9142198
C	-0.4416756	-1.9165924	2.2195674
O	1.3947737	1.2366134	2.0086014
O	-1.0695353	2.0957404	1.3377793
O	0.0412988	-4.1408494	0.4071997
O	-0.3048655	-1.4734260	1.0142599
C	2.1423767	1.8514065	-2.2766320
C	2.4610588	3.0451015	-2.9934816
H	1.9334147	3.9331888	-2.7049744
C	3.3835877	3.0522018	-3.9687787
H	3.6101197	3.9651134	-4.4892234
C	4.0863917	1.8721557	-4.3382260
C	3.7918572	0.6715823	-3.6630251
C	2.8115547	0.6366124	-2.6344819
C	5.0418945	1.8872945	-5.3417969
H	5.2496408	2.8135888	-5.8452915
C	5.7244038	0.7408199	-5.7004952
H	6.4623233	0.7716426	-6.4780838
C	5.4475433	-0.4365391	-5.0504186
H	5.9707466	-1.3362845	-5.3173615
C	4.4897281	-0.4910206	-4.0392102
C	4.1993326	-1.6988572	-3.3643242
H	4.7439006	-2.5854093	-3.6341662
C	3.2640841	-1.7494719	-2.3944253
H	3.0716205	-2.6632427	-1.8620069
C	2.5220238	-0.5990640	-2.0064385
C	-2.2602425	-1.5258242	-3.8303627
C	-2.7816285	-1.9812766	-5.0886449
H	-2.4664236	-2.9563002	-5.4063065
C	-3.6202459	-1.2361418	-5.8193513
H	-3.9975215	-1.6061231	-6.7556669
C	-4.0397851	0.0535180	-5.3843365
C	-3.5494178	0.5483727	-4.1580834
C	-2.6475059	-0.2174801	-3.3635971
C	-4.9108948	0.8130577	-6.1449845
H	-5.2683610	0.4127574	-7.0760059
C	-5.3251662	2.0652645	-5.7292157
H	-6.0023604	2.6390754	-6.3312877
C	-4.8593976	2.5608342	-4.5385023
H	-5.1716127	3.5309031	-4.1975882
C	-3.9781806	1.8240779	-3.7473332
C	-3.5012923	2.3288038	-2.5170577

H	-3.8369131	3.2962532	-2.1900943
C	-2.6461331	1.6201303	-1.7560571
H	-2.3142315	2.0100164	-0.8112234
C	-2.1705201	0.3368603	-2.1511355
O	1.2906181	1.9267741	-1.3509563
O	1.6103307	-0.7594330	-1.1160729
O	-1.5008318	-2.2930258	-3.2003520
O	-1.3210296	-0.2394280	-1.3711732
Sr	-0.2126151	-2.5028645	-1.2541066

#Sr Motif 2,BHLYP-D3

90

Energy = -3341.082667902

Eu	-0.0034056	0.3037979	-2.2127024
C	1.0036712	-2.5506295	-3.5793722
C	1.3400278	-3.1345717	-4.8374129
H	1.2848043	-2.4928385	-5.6949480
C	1.7051097	-4.4230787	-4.9354376
H	1.9532262	-4.8412975	-5.8940943
C	1.7743750	-5.2651293	-3.7921861
C	1.4513686	-4.7234285	-2.5328351
C	1.0620017	-3.3616873	-2.4035551
C	2.1514142	-6.5950597	-3.8997209
H	2.3936012	-6.9876197	-4.8702312
C	2.2197134	-7.4135522	-2.7897165
H	2.5131431	-8.4400023	-2.8916297
C	1.9078216	-6.8979511	-1.5552755
H	1.9562772	-7.5219551	-0.6819002
C	1.5252210	-5.5663926	-1.4094322
C	1.2023681	-5.0266077	-0.1430487
H	1.2552907	-5.6645843	0.7202597
C	0.8329860	-3.7385546	-0.0063256
H	0.5894326	-3.3550351	0.9678856
C	0.7472813	-2.8527736	-1.1180497
C	-2.8856608	0.7385915	-0.4432007
C	-3.5086675	0.6950243	0.8359899
H	-2.9200365	0.3894817	1.6816217
C	-4.8067725	1.0160889	1.0005326
H	-5.2461524	0.9758829	1.9807538
C	-5.6173738	1.4067139	-0.0910916
C	-5.0378955	1.4469451	-1.3716695
C	-3.6690854	1.1121361	-1.5658188
C	-6.9581826	1.7406056	0.0815524
H	-7.3782236	1.7022384	1.0698308
C	-7.7393627	2.1135105	-0.9859623
H	-8.7708418	2.3691823	-0.8414534
C	-7.1818521	2.1542744	-2.2479156
H	-7.7828990	2.4428993	-3.0905904
C	-5.8501686	1.8277408	-2.4573062
C	-5.2772153	1.8664927	-3.7570388
H	-5.9009993	2.1573235	-4.5827841
C	-3.9890131	1.5485889	-3.9654736
H	-3.5489599	1.5731372	-4.9432517
C	-3.1351054	1.1605166	-2.8903588
O	0.6667118	-1.3343414	-3.5642020

O	0.3895388	-1.6419991	-0.8868522
O	-1.6370055	0.4345554	-0.5073107
O	-1.9352555	0.8737980	-3.1651619
C	2.1415287	1.9916175	-0.1703054
C	2.6929695	2.0949476	1.1378221
H	2.3442032	1.4160145	1.8946630
C	3.6406787	3.0057436	1.4342840
H	4.0354675	3.0592327	2.4326585
C	4.1376489	3.9013800	0.4585285
C	3.6261330	3.8156599	-0.8485444
C	2.6292391	2.8575806	-1.1820226
C	5.1129033	4.8461768	0.7678244
H	5.4893952	4.8917385	1.7731938
C	5.5920439	5.7096720	-0.1879198
H	6.3425855	6.4340140	0.0615064
C	5.0967887	5.6346358	-1.4741906
H	5.4637936	6.3046466	-2.2298791
C	4.1268452	4.7050919	-1.8187808
C	3.6184520	4.6257971	-3.1435353
H	4.0026122	5.3075936	-3.8805109
C	2.6824806	3.7244405	-3.4833164
H	2.2965023	3.6553311	-4.4815903
C	2.1545919	2.8042806	-2.5290291
C	1.2223384	-0.3933621	4.4548946
C	2.4155804	-0.3043165	5.2444903
H	3.3347593	-0.1764053	4.7053338
C	2.3894987	-0.3812242	6.5839160
H	3.3024545	-0.3113822	7.1477247
C	1.1703066	-0.5575287	7.2915326
C	-0.0271753	-0.6541573	6.5550584
C	-0.0239847	-0.5751698	5.1338125
C	1.1480106	-0.6364374	8.6776447
H	2.0756803	-0.5603341	9.2149642
C	-0.0335477	-0.8093296	9.3640304
H	-0.0359976	-0.8685175	10.4350128
C	-1.2118797	-0.9059697	8.6573407
H	-2.1418463	-1.0418124	9.1786627
C	-1.2278360	-0.8319684	7.2709042
C	-2.4430083	-0.9347428	6.5422198
H	-3.3576929	-1.0732849	7.0902854
C	-2.4626046	-0.8651086	5.2023906
H	-3.3777480	-0.9480310	4.6478969
C	-1.2670494	-0.6812492	4.4329079
O	1.2205744	1.1128507	-0.3600575
O	1.2873881	1.9754626	-2.9259446
O	1.3414413	-0.3060978	3.2013072
O	-1.3813009	-0.6250460	3.1770673