

Supporting Information

Modeling microsolvation clusters with electronic-structure calculations guided by analytical potentials and predictive machine learning techniques

W.S. Jesus,[†] F.V. Prudente,[†] J.M.C. Marques,^{*,‡} and F.B. Pereira[¶]

[†]*Instituto de Física, Universidade Federal da Bahia, 40170-115 Salvador, BA, Brazil*

[‡]*CQC, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal*

[¶]*Coimbra Polytechnic – ISEC, Coimbra, Portugal*

[§]*Centro de Informática e Sistemas da Universidade de Coimbra (CISUC), Coimbra,
Portugal*

E-mail: qtmarque@ci.uc.pt

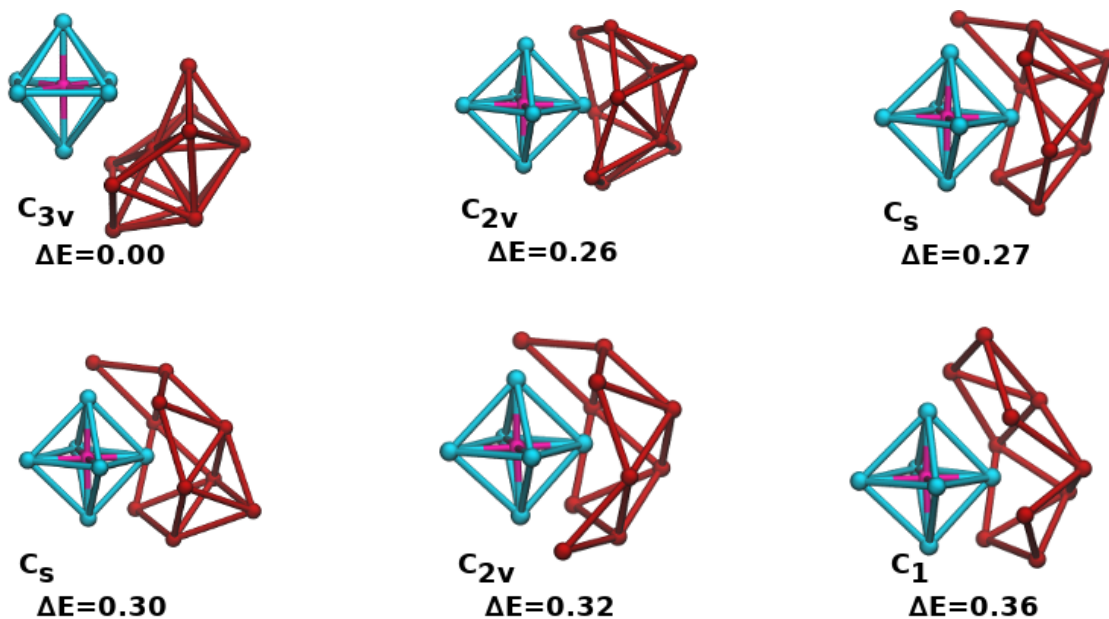


Figure S1: First six lowest-energy minima structures of the $\text{Li}^+\text{Kr}_{16}$ cluster. First (second) solvation shell krypton atoms are in cyan (brown) to highlight its rigidity (fluid-like) character. Also indicated are the corresponding point group of symmetry and the energy difference in relation to the global minimum. Energies are in mEh.

Table S1: Selected features of all Li^+Kr_n structures used in Machine Learning. Specifically, the following attributes are shown in the Table: N and n : number of total and krypton atoms, respectively; Sym: number of symmetry operations; ρ : hyperradius; ξ^- and ξ^+ : deformation indices; E_{PES} : potential energy in mE_h obtained from the analytical PES through the application of the EA; E_{DFT}^{SP} : single point DFT energy in E_h at the PES geometry; Gmax and Grms: the maximum and root mean square gradient in the Cartesian coordinates (in atomic units) of the PES geometry; CN_x ($x = 3-8$): number of atoms with x nearest-neighbors (in %). Additionally, it is shown the re-optimized B3LYP-D3/aug-pseg-1 (DFT) energies from the respective global one (ΔE_{DFT}^{Opt}) in mE_h . Also shown in the last column is the classification labels “P” and “U” for promising and unpromising structures, respectively.

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 8; n = 7$															
6	-55.239	34.05	5.19E-07	-3.15E-01	0.012	-19281.68359	1.17E-03	5.50E-04	12.5	0	37.5	50	0	0	P
2	-54.882	36.21	2.22E-03	-3.54E-01	0.841	-19281.67726	1.10E-03	5.10E-04	0	0	50	37.5	0	0	U
8	-54.388	42.49	2.19E-06	-4.48E-01	1.736	-19281.68199	1.07E-03	4.90E-04	0	0	62.5	25	0	0	U
4	-52.999	34.11	1.91E-01	-1.44E-01	0.159	-19281.67978	1.50E-03	6.10E-04	12.5	25	62.5	0	0	0	P
2	-52.782	38.32	8.00E-03	-4.14E-01	0.022	-19281.67814	1.71E-03	5.90E-04	12.5	37.5	12.5	37.5	0	0	P
4	-52.663	38.43	2.55E-03	-4.23E-01	4.814	-19281.67859	1.57E-03	6.30E-04	25	0	62.5	0	12.5	0	U
2	-52.365	39.51	4.95E-02	-3.86E-01	6.015	-19281.67726	2.03E-03	6.40E-04	37.5	37.5	12.5	12.5	0	0	U
2	-52.333	40.83	5.15E-02	-3.59E-01	0.000	-19281.67742	1.64E-03	6.10E-04	0	37.5	37.5	0	12.5	0	P
2	-52.301	44.04	6.26E-02	-5.66E-01	0.002	-19281.67753	1.66E-03	6.80E-04	12.5	0	62.5	12.5	0	0	P

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 9; n = 8$															
2	-57.515	39.32	9.31E-02	-2.98E-01	0.006	-22035.16341	1.01E-03	4.00E-04	11.1	11.1	33.3	22.2	22.2	0	U
4	-57.419	38.50	1.76E-01	-1.18E-01	0.004	-22035.16367	1.00E-03	3.90E-04	22.2	0	22.2	33.3	22.2	0	P
4	-57.410	38.70	1.02E-01	-2.66E-01	0.007	-22035.16351	1.03E-03	4.00E-04	22.2	0	44.4	11.1	22.2	0	P
12	-57.371	42.30	5.04E-07	-5.19E-01	1.780	-22035.16347	1.13E-03	4.90E-04	22.2	0	0	77.8	0	0	P
4	-57.370	40.43	1.37E-01	-2.22E-01	1.751	-22035.16350	1.01E-03	4.50E-04	22.2	0	11.1	55.6	11.1	0	P
2	-57.195	40.84	8.90E-02	-3.24E-01	2.582	-22035.16267	1.22E-03	4.10E-04	22.2	0	33.3	33.3	11.1	0	U
2	-57.080	43.54	6.71E-02	-3.96E-01	2.798	-22035.16249	1.07E-03	4.20E-04	0	11.1	33.3	33.3	11.1	0	U
1	-57.073	42.94	7.08E-02	-3.83E-01	0.005	-22035.16248	1.11E-03	4.10E-04	0	11.1	33.3	33.3	11.1	0	P
1	-57.019	41.48	2.10E-01	-8.80E-02	2.507	-22035.16277	1.05E-03	3.90E-04	11.1	0	22.2	44.4	11.1	0	U
2	-57.017	43.91	4.07E-02	-4.57E-01	2.479	-22035.16271	1.04E-03	4.60E-04	11.1	0	11.1	66.7	0	0	U
1	-56.530	49.22	8.84E-02	-4.07E-01	3.467	-22035.16183	1.07E-03	4.50E-04	11.1	0	22.2	55.6	0	0	U
2	-55.372	39.92	2.56E-01	-1.05E-01	0.029	-22035.15915	1.71E-03	4.20E-04	0	66.7	11.1	11.1	11.1	0	P
2	-55.339	40.49	8.31E-02	-3.06E-01	1.946	-22035.15916	1.70E-03	4.30E-04	22.2	0	66.7	11.1	0	0	U
2	-55.240	40.91	6.71E-02	-3.34E-01	0.000	-22035.15797	1.51E-03	4.10E-04	0	55.6	11.1	22.2	11.1	0	P

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 10; n = 9$															
6	-59.983	43.61	9.19E-07	-3.65E-01	2.294	-24788.64309	9.20E-04	2.80E-04	0	30	30	10	30	0	U
1	-59.890	45.65	1.76E-02	-4.04E-01	0.603	-24788.64292	1.01E-03	2.80E-04	10	10	40	20	10	10	P
1	-59.813	43.75	2.09E-01	-1.42E-01	0.000	-24788.64319	1.17E-03	3.00E-04	10	20	20	30	10	10	P
2	-59.793	43.51	1.73E-01	-1.50E-01	0.000	-24788.64320	1.04E-03	2.80E-04	20	0	40	10	20	10	P
2	-59.792	44.41	1.16E-01	-2.93E-01	2.010	-24788.64321	1.11E-03	2.90E-04	10	20	20	30	10	10	U
2	-59.787	45.25	2.69E-02	-3.90E-01	0.604	-24788.64300	1.12E-03	3.00E-04	10	20	40	10	10	10	P
4	-59.730	43.68	2.10E-01	-1.70E-01	2.243	-24788.64307	1.22E-03	3.10E-04	0	10	20	50	0	0	U
1	-59.691	43.39	1.92E-01	-1.26E-01	0.211	-24788.64328	1.06E-03	2.80E-04	20	10	30	20	10	10	P
1	-59.684	43.45	1.81E-01	-9.94E-02	1.550	-24788.64352	1.07E-03	2.80E-04	20	10	20	20	20	10	P
1	-59.638	44.48	1.56E-01	-1.59E-01	0.211	-24788.64336	1.04E-03	2.90E-04	20	10	10	40	10	10	P
2	-59.633	47.92	8.46E-02	-4.55E-01	1.705	-24788.64330	1.03E-03	3.00E-04	20	10	0	50	20	0	U
2	-59.633	46.94	1.16E-01	-3.85E-01	1.705	-24788.64325	1.04E-03	3.90E-04	20	10	10	30	30	0	U
2	-59.587	47.21	1.16E-02	-4.21E-01	3.264	-24788.64218	9.60E-04	2.90E-04	10	20	30	30	0	10	U
2	-59.577	43.14	1.52E-01	-7.69E-02	1.404	-24788.64371	9.70E-04	2.90E-04	30	0	10	30	20	10	P
2	-59.532	46.13	1.48E-01	-3.11E-01	1.715	-24788.64355	9.40E-04	3.00E-04	30	0	0	40	30	0	U
6	-59.482	46.15	2.33E-01	-1.80E-06	1.962	-24788.64341	1.04E-03	2.90E-04	30	0	0	40	30	0	U
2	-59.357	47.71	2.41E-01	-1.39E-01	1.217	-24788.64227	1.17E-03	2.90E-04	10	0	40	10	30	0	P

2	-59.222	47.66	2.36E-01	-1.47E-01	2.937	-24788.64240	1.02E-03	3.00E-04	10	10	10	50	0	10	U
2	-59.205	52.37	6.91E-02	-5.15E-01	3.133	-24788.64225	1.01E-03	3.90E-04	10	10	0	60	10	0	U
1	-59.203	50.23	5.71E-02	-3.97E-01	3.061	-24788.64234	1.02E-03	3.10E-04	10	10	10	40	20	0	U
1	-58.073	43.73	1.59E-01	-2.23E-01	1.611	-24788.63935	1.77E-03	2.70E-04	10	20	40	20	10	0	P
1	-58.012	45.67	1.41E-01	-2.86E-01	1.579	-24788.63821	1.68E-03	2.70E-04	0	50	10	20	10	10	P
2	-57.958	44.02	1.58E-01	-1.87E-01	0.011	-24788.63840	1.58E-03	2.60E-04	0	50	10	30	0	0	P
1	-57.917	43.16	2.20E-01	-1.24E-01	1.670	-24788.64019	1.64E-03	2.50E-04	0	40	40	0	20	0	U
1	-57.766	45.35	1.61E-01	-2.40E-01	0.603	-24788.63871	1.62E-03	2.60E-04	10	40	30	10	0	10	P
1	-57.691	45.03	2.18E-01	-7.43E-02	1.406	-24788.63885	1.53E-03	2.70E-04	10	40	30	10	0	10	P
2	-57.700	40.91	6.71E-02	-3.34E-01	7.483	-24788.63751	1.73E-03	2.80E-04	10	30	30	20	0	10	U
1	-57.646	45.83	2.18E-01	-6.63E-02	2.354	-24788.63877	1.78E-03	2.70E-04	30	0	30	40	0	0	U
2	-57.603	45.20	1.46E-01	-1.08E-01	2.354	-24788.63903	1.71E-03	2.70E-04	30	0	40	20	10	0	U

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Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 11; n = 10$															
2	-62.692	47.65	1.12E-01	-2.83E-01	1.535	-27542.12342	1.07E-03	1.90E-04	0	27.3	27.3	18.2	18.2	0	P
4	-62.682	47.73	6.83E-02	-3.43E-01	1.572	-27542.12341	8.90E-04	1.90E-04	0	18.2	36.4	27.3	0	18.2	P
2	-62.594	46.36	1.53E-01	-1.58E-01	1.339	-27542.12361	1.00E-03	1.80E-04	0	27.3	27.3	18.2	9.1	18.2	P
2	-62.413	47.07	2.59E-01	-8.12E-03	1.200	-27542.12370	1.17E-03	1.90E-04	0	36.4	9.1	27.3	18.2	0	P
2	-62.383	49.17	1.05E-01	-2.81E-01	2.459	-27542.12262	1.21E-03	2.00E-04	9.1	9.1	45.5	9.1	18.2	9.1	U

2	-62.279	50.44	1.02E-01	-2.95E-01	2.485	-27542.12248	1.05E-03	1.90E-04	18.2	0	36.4	27.3	0	18.2	U
1	-62.187	49.34	1.77E-01	-1.76E-01	2.284	-27542.12268	1.22E-03	2.00E-04	18.2	0	36.4	27.3	0	18.2	U
1	-62.168	49.36	1.60E-01	-1.82E-01	1.915	-27542.12278	1.08E-03	1.90E-04	18.2	9.1	27.3	18.2	9.1	18.2	U
2	-62.094	49.60	1.05E-01	-2.89E-01	2.048	-27542.12306	1.07E-03	2.00E-04	9.1	27.3	9.1	27.3	18.2	9.1	U
6	-62.094	53.21	5.83E-07	-5.32E-01	2.169	-27542.12294	1.07E-03	2.00E-04	9.1	27.3	9.1	27.3	18.2	9.1	U
1	-61.994	54.60	2.46E-03	-5.38E-01	2.808	-27542.12202	1.14E-03	2.00E-04	9.1	9.1	36.4	27.3	9.1	9.1	U
4	-61.885	54.78	1.07E-01	-4.92E-01	1.721	-27542.12306	9.00E-04	3.10E-04	18.2	18.2	0	27.3	36.4	0	P
1	-61.784	50.76	1.13E-01	-3.23E-01	1.005	-27542.12345	9.80E-04	2.20E-04	27.3	9.1	0	27.3	27.3	9.1	P
2	-61.698	49.96	7.91E-03	-3.10E-01	2.700	-27542.12230	1.06E-03	1.90E-04	0	27.3	18.2	27.3	9.1	0	U
1	-61.650	52.70	2.50E-01	-1.52E-01	2.919	-27542.12245	1.23E-03	2.20E-04	9.1	9.1	27.3	18.2	18.2	9.1	U
2	-61.485	53.06	2.96E-01	-1.03E-01	2.459	-27542.12226	1.08E-03	2.20E-04	18.2	0	18.2	27.3	18.2	9.1	U
2	-61.374	54.27	1.87E-01	-3.24E-01	2.449	-27542.12252	9.10E-04	2.20E-04	18.2	9.1	0	36.4	18.2	9.1	U
2	-60.699	47.75	1.34E-01	-1.80E-01	0.746	-27542.11902	1.48E-03	6.20E-04	0	45.5	27.3	9.1	9.1	9.1	P
2	-60.548	46.88	2.48E-01	-3.27E-03	5.184	-27542.11942	1.29E-03	5.90E-04	0	27.3	45.5	0	18.2	0	U
1	-60.451	49.00	2.02E-01	-1.46E-01	1.811	-27542.11882	1.61E-03	6.50E-04	18.2	9.1	45.5	0	27.3	0	U
1	-60.220	50.04	1.47E-01	-2.90E-01	1.812	-27542.11855	1.61E-03	6.50E-04	18.2	9.1	36.4	18.2	18.2	0	U
1	-60.033	51.90	1.29E-01	-2.66E-01	2.026	-27542.11712	1.66E-03	6.30E-04	9.1	27.3	36.4	18.2	0	0	U
1	-62.080	48.56	2.57E-01	-7.58E-02	0.000	-27542.12301	1.12E-03	2.10E-04	18.2	9.1	27.3	18.2	9.1	18.2	P
6	-62.072	46.90	2.47E-05	-1.46E-01	1.628	-27542.12315	8.70E-04	1.70E-04	27.3	0	27.3	18.2	0	27.3	P
6	-62.071	52.87	5.39E-07	-5.28E-01	2.961	-27542.12213	9.20E-04	1.90E-04	9.1	0	54.5	9.1	27.3	0	U
1	-62.024	49.35	1.48E-01	-2.00E-01	1.891	-27542.12298	1.09E-03	1.90E-04	18.2	9.1	18.2	36.4	9.1	0	U

1	-62.006	51.40	1.06E-01	-3.23E-01	2.000	-27542.12286	1.00E-03	2.00E-04	18.2	9.1	18.2	36.4	0	18.2	U
1	-62.001	54.80	2.49E-02	-5.16E-01	2.166	-27542.12276	1.01E-03	2.80E-04	18.2	9.1	9.1	45.5	9.1	9.1	U
1	-62.000	53.53	6.56E-02	-4.39E-01	2.118	-27542.12280	9.30E-04	2.20E-04	18.2	9.1	18.2	27.3	18.2	9.1	U
1	-61.926	48.03	1.07E-01	-9.82E-02	1.817	-27542.12317	1.09E-03	1.80E-04	18.2	18.2	9.1	27.3	9.1	18.2	U
1	-61.919	51.22	1.95E-01	-2.70E-01	0.357	-27542.12310	1.11E-03	2.30E-04	18.2	18.2	0	36.4	18.2	9.1	P
1	-61.918	51.97	1.59E-01	-3.39E-01	1.957	-27542.12306	1.10E-03	2.50E-04	18.2	18.2	0	36.4	18.2	9.1	U
1	-61.902	49.78	1.76E-01	-2.22E-01	1.574	-27542.12317	1.00E-03	2.00E-04	27.3	0	18.2	27.3	9.1	18.2	P
2	-61.900	48.26	8.61E-02	-1.41E-01	1.471	-27542.12333	9.50E-04	1.80E-04	18.2	18.2	9.1	27.3	18.2	0	P
2	-61.830	47.57	9.01E-02	-2.48E-02	1.238	-27542.12356	1.03E-03	1.80E-04	27.3	9.1	9.1	27.3	0	27.3	P
2	-61.742	49.20	1.01E-01	-6.14E-02	1.089	-27542.12338	9.50E-04	1.70E-04	27.3	9.1	0	36.4	9.1	18.2	P
2	-61.718	48.77	1.25E-01	-2.22E-01	1.046	-27542.12386	9.10E-04	1.80E-04	36.4	0	0	27.3	18.2	18.2	P
2	-61.670	50.01	1.76E-01	-1.61E-01	1.332	-27542.12369	9.20E-04	2.00E-04	36.4	0	0	18.2	36.4	9.1	P
1	-61.667	52.26	2.49E-01	-1.44E-01	2.895	-27542.12204	9.30E-04	2.10E-04	0	27.3	18.2	18.2	18.2	9.1	U
1	-61.467	54.59	9.25E-02	-3.49E-01	2.345	-27542.12221	1.02E-03	2.40E-04	9.1	18.2	9.1	27.3	18.2	9.1	U
2	-60.693	48.46	1.73E-01	-2.31E-01	0.063	-27542.11888	1.59E-03	1.70E-04	0	45.5	27.3	18.2	0	0	P
2	-60.678	46.78	1.90E-01	-9.60E-02	0.814	-27542.11945	1.65E-03	6.60E-04	18.2	0	36.4	18.2	0	9.1	P
1	-60.677	46.13	2.33E-01	-3.94E-02	0.820	-27542.12013	1.65E-03	6.10E-04	0	27.3	45.5	9.1	9.1	9.1	P
1	-60.512	47.19	1.60E-01	-1.33E-01	1.356	-27542.11837	1.29E-03	6.20E-04	9.1	18.2	45.5	9.1	18.2	0	P
1	-60.510	48.47	5.62E-02	-2.56E-01	1.682	-27542.11910	1.71E-03	6.50E-04	18.2	0	54.5	18.2	0	9.1	P
1	-60.441	48.55	1.69E-01	-8.74E-02	1.418	-27542.11874	1.27E-03	6.40E-04	18.2	27.3	18.2	18.2	18.2	0	P

1	-60.213	51.65	1.25E-01	-3.91E-01	1.597	-27542.11947	1.65E-03	2.00E-04	9.1	27.3	18.2	36.4	9.1	0	P
Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 12; n = 11$															
2	-65.188	49.36	1.56E-01	-5.04E-02	0.853	-30295.60417	1.14E-03	1.20E-04	0	25	25	25	0	16.7	P
1	-65.173	50.21	1.24E-01	-1.99E-01	1.856	-30295.60331	1.11E-03	1.20E-04	0	16.7	41.7	16.7	8.3	16.7	U
1	-65.097	50.94	9.57E-02	-2.30E-01	1.809	-30295.60323	1.08E-03	1.20E-04	8.3	8.3	41.7	16.7	16.7	0	P
1	-65.080	52.43	1.59E-01	-1.69E-01	2.116	-30295.60292	1.13E-03	1.20E-04	8.3	16.7	33.3	8.3	16.7	8.3	U
1	-65.077	51.20	1.20E-01	-2.24E-01	1.913	-30295.60321	9.50E-04	1.20E-04	8.3	8.3	33.3	33.3	0	8.3	U
1	-65.074	50.27	1.49E-01	-1.52E-01	1.609	-30295.60348	1.08E-03	1.20E-04	8.3	16.7	25	25	16.7	0	P
1	-65.041	50.16	1.20E-01	-1.83E-01	1.679	-30295.60334	1.08E-03	1.30E-04	0	16.7	33.3	16.7	16.7	0	P
1	-65.036	50.36	1.83E-01	-1.37E-01	1.461	-30295.60362	1.05E-03	1.20E-04	16.7	8.3	33.3	16.7	16.7	0	P
2	-65.012	51.46	1.20E-01	-2.45E-01	2.232	-30295.60295	1.22E-03	1.40E-04	0	33.3	16.7	33.3	0	16.7	U
1	-65.008	51.36	1.24E-01	-2.33E-01	2.235	-30295.60296	9.00E-04	1.30E-04	0	33.3	16.7	33.3	8.3	0	U
2	-64.900	56.13	6.92E-02	-4.38E-01	2.775	-30295.60236	1.03E-03	1.30E-04	0	33.3	16.7	33.3	8.3	0	U
1	-64.816	55.38	9.55E-02	-4.00E-01	2.525	-30295.60254	1.14E-03	1.30E-04	8.3	8.3	41.7	8.3	25	0	U
2	-64.688	53.05	1.91E-01	-1.92E-01	1.616	-30295.60360	7.90E-04	1.20E-04	8.3	25	8.3	33.3	0	25	P
2	-64.550	53.97	2.02E-01	-6.90E-02	2.679	-30295.60238	8.90E-04	1.20E-04	16.7	16.7	25	8.3	8.3	25	U
2	-64.500	54.48	2.06E-01	-2.04E-01	1.572	-30295.60369	1.14E-03	1.50E-04	8.3	33.3	0	16.7	33.3	0	P
2	-64.315	52.41	1.20E-01	-3.63E-02	1.987	-30295.60299	1.00E-03	1.20E-04	25	0	33.3	8.3	16.7	8.3	U

1	-64.176	52.36	2.39E-02	-1.60E-01	1.907	-30295.60313	1.06E-03	1.20E-04	16.7	25	8.3	16.7	16.7	8.3	U
1	-64.100	57.01	2.14E-01	-2.85E-01	2.023	-30295.60318	1.03E-03	1.80E-04	25	16.7	0	8.3	41.7	8.3	U
1	-63.873	60.42	8.96E-02	-3.21E-01	3.368	-30295.60180	1.07E-03	1.70E-04	0	25	16.7	25	8.3	16.7	U
1	-63.606	48.92	1.74E-01	-7.34E-02	0.955	-30295.60044	1.56E-03	5.90E-04	0	25	41.7	16.7	8.3	0	P
1	-63.264	51.54	1.69E-01	-8.88E-02	0.000	-30295.59916	1.54E-03	6.30E-04	8.3	25	33.3	8.3	8.3	16.7	P
2	-63.195	52.37	2.07E-01	-1.04E-01	1.080	-30295.59902	1.36E-03	6.30E-04	8.3	33.3	8.3	16.7	33.3	0	P
2	-63.049	50.56	1.69E-01	-1.73E-02	0.119	-30295.59856	1.55E-03	6.50E-04	8.3	25	25	25	16.7	0	P
1	-62.896	53.45	1.60E-01	-2.66E-01	0.146	-30295.59767	1.71E-03	6.00E-04	0	33.3	33.3	16.7	8.3	0	P
2	-62.554	55.92	4.17E-02	-9.13E-02	8.204	-30295.59670	1.48E-03	5.90E-04	25	16.7	8.3	25	16.7	8.3	U
2	-64.988	52.58	1.97E-01	-1.74E-01	2.007	-30295.60314	1.20E-03	1.40E-04	8.3	8.3	41.7	16.7	0	25	U
1	-64.794	54.40	1.43E-01	-3.11E-01	1.767	-30295.60335	1.04E-03	1.40E-04	8.3	25	8.3	33.3	8.3	8.3	P
1	-64.794	54.40	1.43E-01	-3.11E-01	1.902	-30295.60320	1.04E-03	1.90E-04	8.3	25	0	41.7	16.7	0	U
2	-64.786	54.00	1.56E-01	-1.57E-01	3.085	-30295.60216	1.17E-03	1.30E-04	16.7	0	41.7	16.7	8.3	16.7	U
2	-64.782	56.52	7.67E-02	-4.48E-01	1.930	-30295.60330	8.90E-04	1.60E-04	8.3	16.7	16.7	33.3	8.3	16.7	U
2	-64.779	56.30	7.46E-02	-4.49E-01	2.656	-30295.60249	8.70E-04	1.20E-04	8.3	0	41.7	33.3	0	16.7	U
2	-64.764	54.28	1.97E-02	-4.37E-01	2.993	-30295.60224	1.19E-03	1.30E-04	0	16.7	50	8.3	16.7	8.3	U
2	-64.687	55.03	1.17E-01	-3.55E-01	2.835	-30295.60232	8.90E-04	1.40E-04	8.3	25	8.3	25	16.7	16.7	U
1	-64.676	50.30	1.13E-01	-4.74E-02	1.147	-30295.60380	7.30E-04	1.10E-04	8.3	25	16.7	16.7	25	0	P
4	-64.549	50.29	1.99E-01	-7.19E-03	2.833	-30295.60232	8.90E-04	1.40E-04	0	33.3	16.7	16.7	16.7	16.7	U
1	-64.549	52.77	2.03E-01	-1.80E-01	1.187	-30295.60382	8.00E-04	1.30E-04	8.3	33.3	0	25	16.7	8.3	P
2	-64.526	54.88	2.61E-01	-6.52E-02	2.835	-30295.60232	8.90E-04	1.40E-04	0	16.7	25	25	8.3	16.7	U

2	-64.507	51.23	8.29E-02	-1.75E-02	1.390	-30295.60378	1.12E-03	1.10E-04	8.3	33.3	0	33.3	0	16.7	P
1	-64.269	55.87	9.51E-02	-2.99E-01	2.211	-30295.60273	8.70E-04	1.40E-04	25	8.3	8.3	33.3	0	25	U
1	-64.252	58.90	7.27E-02	-4.49E-01	1.701	-30295.60268	8.80E-04	1.70E-04	16.7	16.7	16.7	16.7	16.7	16.7	P
1	-64.230	51.83	9.94E-02	-8.54E-02	1.742	-30295.60325	7.80E-04	1.10E-04	25	8.3	16.7	25	0	16.7	P
1	-64.163	56.49	8.60E-02	-3.60E-01	1.966	-30295.60292	1.09E-03	1.80E-04	16.7	25	0	25	16.7	16.7	U
1	-64.144	57.74	9.02E-02	-4.12E-01	1.701	-30295.60295	9.80E-04	1.70E-04	16.7	25	0	25	16.7	16.7	P
1	-64.143	57.12	1.47E-01	-3.58E-01	1.628	-30295.60298	9.30E-04	1.70E-04	25	8.3	16.7	8.3	25	16.7	P
1	-64.127	58.16	1.16E-01	-3.74E-01	3.600	-30295.60162	1.22E-03	1.70E-04	16.7	8.3	16.7	41.7	8.3	0	U
1	-64.053	57.01	2.14E-01	-2.85E-01	2.025	-30295.60318	1.03E-03	1.80E-04	25	16.7	0	8.3	41.7	8.3	U
1	-64.039	57.42	2.23E-01	-1.20E-01	3.600	-30295.60162	1.22E-03	1.70E-04	8.3	8.3	33.3	16.7	8.3	16.7	U
1	-63.564	59.02	1.00E-01	-2.33E-01	0.656	-30295.60218	1.04E-03	1.60E-04	16.7	16.7	0	25	16.7	16.7	P
2	-63.536	50.16	8.19E-02	-1.92E-01	1.370	-30295.59971	1.74E-03	6.30E-04	8.3	25	33.3	25	0	0	P
1	-63.264	51.54	1.69E-01	-8.88E-02	1.370	-30295.59916	1.54E-03	6.30E-04	8.3	25	33.3	8.3	8.3	16.7	P
1	-63.245	51.65	2.39E-01	-8.54E-02	1.214	-30295.59879	1.40E-03	6.10E-04	0	41.7	8.3	33.3	0	8.3	P
1	-63.148	52.74	1.50E-01	-2.19E-01	1.374	-30295.59866	1.36E-03	6.20E-04	8.3	25	25	16.7	16.7	8.3	P
1	-63.148	52.74	1.50E-01	-2.19E-01	1.166	-30295.59893	1.40E-03	6.30E-04	25	0	25	8.3	16.7	8.3	P
2	-63.011	51.77	6.86E-04	-2.53E-01	1.697	-30295.59802	1.24E-03	5.80E-04	0	16.7	50	0	0	16.7	P

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
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$N = 13; n = 12$

2	-68.011	53.02	1.17E-02	-2.49E-01	1.747	-33049.08377	1.27E-03	4.60E-04	0	15.4	38.5	23.1	15.4	0	P
1	-67.897	53.43	1.65E-01	-1.46E-01	1.462	-33049.08398	1.04E-03	4.50E-04	0	7.7	46.2	30.8	7.7	0	P
2	-67.872	54.14	1.23E-01	-1.06E-01	0.000	-33049.08352	1.03E-03	4.50E-04	0	30.8	30.8	7.7	0	15.4	P
2	-67.853	52.29	1.77E-02	-2.23E-01	0.592	-33049.08383	1.30E-03	4.60E-04	0	23.1	46.2	15.4	7.7	0	P
1	-67.844	53.40	2.31E-01	-2.88E-02	1.574	-33049.08393	1.13E-03	4.60E-04	0	30.8	15.4	23.1	15.4	7.7	P
2	-67.813	53.50	1.90E-01	-1.09E-01	1.622	-33049.08398	1.27E-03	4.50E-04	0	15.4	38.5	23.1	15.4	0	P
1	-67.763	52.38	5.61E-02	-1.30E-01	1.432	-33049.08406	1.24E-03	4.50E-04	0	23.1	23.1	23.1	0	15.4	P
2	-67.763	52.40	6.12E-02	-1.24E-01	1.387	-33049.08421	1.12E-03	4.50E-04	7.7	23.1	7.7	38.5	0	15.4	P
6	-67.762	52.40	1.24E-05	-4.44E-02	0.705	-33049.08482	1.08E-03	4.30E-04	0	23.1	23.1	30.8	0	0	P
1	-67.752	52.89	1.16E-01	-1.27E-01	1.370	-33049.08403	1.26E-03	4.60E-04	0	23.1	23.1	30.8	15.4	0	P
1	-67.617	55.47	2.56E-01	-1.92E-02	0.765	-33049.08308	1.08E-03	4.50E-04	0	30.8	15.4	38.5	0	0	P
1	-67.493	56.00	1.02E-01	-3.05E-01	2.207	-33049.08278	1.18E-03	4.40E-04	0	23.1	23.1	38.5	7.7	0	U
2	-67.287	56.91	1.24E-01	-2.44E-01	3.153	-33049.08336	1.16E-03	4.50E-04	7.7	15.4	15.4	38.5	0	15.4	U
1	-67.199	59.02	9.07E-02	-3.57E-01	1.760	-33049.08234	1.16E-03	4.40E-04	7.7	15.4	23.1	30.8	15.4	0	U
1	-67.044	60.41	1.30E-01	-3.40E-01	2.487	-33049.08245	1.16E-03	4.40E-04	7.7	15.4	23.1	30.8	15.4	0	U
1	-66.977	55.49	6.34E-02	-1.43E-01	3.321	-33049.08288	1.01E-03	4.40E-04	23.1	7.7	7.7	38.5	0	7.7	U
2	-66.876	65.25	1.02E-01	-4.80E-01	3.092	-33049.08237	1.09E-03	4.10E-04	15.4	0	23.1	38.5	7.7	15.4	U
1	-66.800	57.16	9.37E-02	-2.25E-01	3.108	-33049.08378	8.30E-04	1.00E-04	7.7	38.5	0	15.4	23.1	0	P
2	-66.663	62.82	6.28E-02	-4.23E-01	0.473	-33049.08241	1.03E-03	1.20E-04	15.4	15.4	30.8	7.7	7.7	15.4	U
1	-66.533	50.54	1.00E-01	-4.67E-02	1.289	-33049.08241	1.03E-03	1.20E-04	0	23.1	38.5	23.1	7.7	0	U
2	-66.138	54.48	4.59E-02	-6.37E-02	1.637	-33049.07856	1.61E-03	5.80E-04	0	38.5	30.8	0	0	15.4	P

4	-65.977	53.53	1.05E-02	-2.49E-02	1.637	-33049.07877	1.73E-03	6.20E-04	7.7	15.4	38.5	15.4	15.4	7.7	P
1	-65.416	54.83	9.13E-02	-1.94E-01	1.637	-33049.08084	1.39E-03	5.50E-04	7.7	23.1	30.8	23.1	0	7.7	P
1	-67.742	53.85	1.66E-01	-1.40E-01	1.766	-33049.08385	9.20E-04	4.50E-04	0	15.4	38.5	23.1	0	15.4	P
1	-67.707	57.47	1.29E-01	-3.11E-01	2.685	-33049.08287	1.06E-03	4.50E-04	0	23.1	30.8	15.4	7.7	15.4	U
1	-67.561	56.93	2.04E-01	-2.25E-01	1.653	-33049.08379	8.50E-04	4.40E-04	0	30.8	15.4	23.1	15.4	0	P
2	-67.487	60.46	1.01E-01	-4.37E-01	3.259	-33049.08228	1.05E-03	4.40E-04	0	15.4	38.5	15.4	15.4	7.7	U
1	-67.480	56.16	2.38E-01	-3.06E-02	2.738	-33049.08276	1.04E-03	4.40E-04	15.4	0	46.2	7.7	15.4	7.7	U
2	-67.448	51.74	5.35E-02	-1.28E-01	2.075	-33049.08416	1.19E-03	4.50E-04	0	38.5	15.4	30.8	7.7	0	P
1	-67.302	57.46	9.85E-02	-3.50E-01	3.157	-33049.08251	1.05E-03	4.50E-04	7.7	7.7	30.8	30.8	7.7	15.4	U
2	-67.264	57.23	1.31E-01	-2.96E-01	0.965	-33049.08274	1.20E-03	4.50E-04	0	23.1	30.8	23.1	0	23.1	P
2	-67.262	57.24	2.84E-01	-8.30E-02	2.579	-33049.08308	8.90E-04	4.40E-04	15.4	7.7	23.1	30.8	0	15.4	U
1	-67.258	57.53	1.17E-01	-2.99E-01	2.428	-33049.08330	1.03E-03	4.20E-04	7.7	15.4	23.1	30.8	0	23.1	U
1	-67.256	59.20	1.05E-01	-3.61E-01	2.474	-33049.08326	1.09E-03	1.10E-04	7.7	15.4	23.1	23.1	15.4	15.4	U
1	-67.229	57.82	1.27E-01	-2.73E-01	3.101	-33049.08237	1.13E-03	4.50E-04	15.4	0	38.5	15.4	23.1	0	U
1	-67.183	59.52	7.98E-02	-3.53E-01	2.440	-33049.08305	1.03E-03	1.30E-04	15.4	7.7	15.4	38.5	15.4	0	U
1	-67.031	59.40	1.30E-01	-2.98E-01	2.351	-33049.08312	8.20E-04	1.00E-04	7.7	30.8	7.7	23.1	7.7	15.4	U
1	-67.030	59.76	1.50E-01	-3.24E-01	2.299	-33049.08307	1.21E-03	1.20E-04	15.4	7.7	30.8	15.4	7.7	15.4	U
1	-66.970	58.89	3.99E-02	-3.44E-01	1.150	-33049.08264	1.03E-03	4.40E-04	15.4	7.7	30.8	15.4	7.7	15.4	P
1	-66.860	60.53	2.53E-01	-1.45E-01	2.484	-33049.08322	1.16E-03	1.20E-04	15.4	15.4	15.4	15.4	23.1	7.7	U
2	-66.852	62.63	1.22E-01	-4.30E-01	4.673	-33049.08105	1.14E-03	4.30E-04	0	23.1	30.8	7.7	30.8	7.7	U
1	-66.782	57.16	9.37E-02	-2.25E-01	1.695	-33049.08378	8.30E-04	1.00E-04	7.7	38.5	0	15.4	23.1	0	P

1	-66.754	56.53	1.29E-01	-1.50E-01	1.405	-33049.08380	1.00E-03	4.10E-04	15.4	23.1	7.7	15.4	23.1	7.7	P
1	-66.521	63.96	6.46E-02	-4.28E-01	3.069	-33049.08241	1.09E-03	1.50E-04	15.4	23.1	7.7	23.1	7.7	23.1	U
2	-66.090	66.11	6.35E-02	-3.74E-01	2.555	-33049.08175	1.05E-03	4.20E-04	7.7	23.1	0	38.5	15.4	0	U

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 14; n = 13$															
2	-71.183	54.10	8.66E-02	-1.37E-01	0.666	-35802.56525	1.54E-03	4.60E-04	0	0	42.9	35.7	14.3	0	P
6	-70.765	56.84	1.09E-05	-1.19E-01	2.113	-35802.56371	1.16E-03	4.40E-04	0	21.4	42.9	7.1	0	0	P
2	-70.639	57.27	2.47E-01	-1.29E-02	1.779	-35802.56412	9.80E-04	4.40E-04	0	28.6	28.6	14.3	21.4	0	P
1	-70.632	54.94	1.52E-01	-7.78E-02	0.823	-35802.56475	1.20E-03	4.50E-04	0	28.6	28.6	14.3	21.4	0	P
2	-70.607	54.86	1.52E-01	-8.08E-02	0.768	-35802.56475	1.12E-03	4.50E-04	0	14.3	42.9	21.4	14.3	0	P
2	-70.588	55.56	5.85E-02	-9.79E-02	1.493	-35802.56448	1.32E-03	4.50E-04	0	21.4	21.4	35.7	0	14.3	P
2	-70.566	58.01	1.56E-01	-2.30E-01	2.110	-35802.56392	1.24E-03	4.30E-04	0	7.1	35.7	35.7	14.3	0	P
1	-70.545	56.29	1.82E-01	-3.54E-02	2.030	-35802.56404	1.26E-03	4.40E-04	0	21.4	21.4	35.7	7.1	7.1	P
2	-70.526	54.02	2.68E-02	-7.12E-02	0.803	-35802.56507	1.37E-03	4.60E-04	0	21.4	28.6	14.3	28.6	0	P
4	-70.471	53.80	7.84E-02	-6.29E-02	1.162	-35802.56468	9.40E-04	4.50E-04	0	28.6	28.6	35.7	0	0	P
2	-70.457	58.68	9.30E-02	-2.49E-01	0.513	-35802.56338	1.11E-03	4.40E-04	0	21.4	35.7	14.3	0	7.1	P
1	-70.279	58.92	2.47E-01	-3.93E-02	1.002	-35802.56356	1.39E-03	4.40E-04	7.1	7.1	28.6	42.9	0	7.1	P
1	-70.148	58.72	1.10E-01	-1.27E-01	2.440	-35802.56344	1.01E-03	4.40E-04	7.1	21.4	28.6	14.3	0	7.1	U
1	-69.981	59.69	1.33E-01	-2.60E-01	1.810	-35802.56379	1.04E-03	4.30E-04	7.1	7.1	42.9	14.3	7.1	7.1	P

1	-69.879	60.84	1.49E-01	-2.64E-01	2.800	-35802.56304	1.08E-03	4.30E-04	7.1	7.1	28.6	35.7	0	14.3	U
1	-69.716	58.82	8.07E-02	-1.95E-01	1.631	-35802.56417	9.50E-04	4.40E-04	7.1	21.4	28.6	7.1	7.1	21.4	P
2	-69.584	60.56	1.61E-02	-1.62E-01	3.208	-35802.56273	1.09E-03	4.20E-04	21.4	7.1	21.4	21.4	0	21.4	U
1	-69.418	66.20	8.38E-02	-4.17E-01	2.890	-35802.56293	9.40E-04	4.10E-04	14.3	14.3	21.4	14.3	21.4	7.1	U
4	-69.297	64.35	1.37E-01	-3.32E-01	2.673	-35802.56175	9.90E-04	4.40E-04	14.3	0	42.9	14.3	0	28.6	U
1	-68.944	62.54	9.44E-02	-2.17E-01	3.734	-35802.56230	1.24E-03	4.40E-04	7.1	28.6	14.3	7.1	14.3	14.3	U
1	-68.856	60.15	4.99E-02	-1.59E-01	1.405	-35802.56391	8.70E-04	3.90E-04	14.3	35.7	0	14.3	14.3	14.3	P
2	-68.641	58.27	1.59E-01	-3.13E-02	1.629	-35802.55921	1.62E-03	5.80E-04	7.1	35.7	21.4	7.1	7.1	14.3	P
1	-68.596	66.20	1.90E-01	-2.48E-01	3.141	-35802.56264	9.00E-04	3.90E-04	28.6	14.3	0	21.4	7.1	21.4	U
1	-70.418	56.04	5.95E-02	-1.26E-01	1.903	-35802.56386	1.18E-03	4.40E-04	0	28.6	14.3	35.7	7.1	7.1	P
1	-70.414	57.74	1.84E-01	-1.56E-01	1.379	-35802.56455	1.08E-03	4.40E-04	0	28.6	14.3	28.6	7.1	7.1	P
1	-70.346	56.71	1.50E-01	-3.30E-02	2.213	-35802.56362	1.05E-03	4.40E-04	0	28.6	14.3	21.4	14.3	7.1	P
1	-70.329	55.98	3.99E-02	-1.25E-01	1.233	-35802.56465	1.08E-03	4.30E-04	0	21.4	21.4	28.6	0	0	P
1	-70.320	61.94	1.34E-01	-3.32E-01	3.361	-35802.56261	1.15E-03	4.40E-04	0	14.3	35.7	21.4	7.1	7.1	U
1	-70.270	57.73	1.32E-01	-4.82E-02	2.489	-35802.56337	1.12E-03	4.40E-04	7.1	21.4	28.6	14.3	0	14.3	U
1	-70.230	59.93	1.83E-01	-1.69E-01	2.505	-35802.56345	1.13E-03	4.40E-04	7.1	14.3	28.6	21.4	7.1	14.3	U
1	-70.136	59.96	4.14E-02	-3.22E-01	2.993	-35802.56294	1.46E-03	4.40E-04	7.1	7.1	35.7	21.4	21.4	0	U
2	-70.087	61.17	2.85E-02	-3.34E-01	2.340	-35802.56360	1.14E-03	4.10E-04	7.1	14.3	14.3	42.9	14.3	0	U
1	-70.060	60.83	1.93E-01	-2.11E-01	3.090	-35802.56293	1.20E-03	4.40E-04	7.1	14.3	28.6	21.4	7.1	14.3	U
4	-69.953	50.94	5.43E-02	-2.98E-03	0.000	-35802.56330	1.20E-03	4.40E-04	0	14.3	64.3	14.3	0	0	P
1	-69.938	62.31	1.54E-01	-2.50E-01	2.508	-35802.56334	1.14E-03	4.20E-04	7.1	21.4	21.4	14.3	14.3	7.1	U

1	-69.928	59.25	5.63E-02	-2.33E-01	3.520	-35802.56249	1.26E-03	4.30E-04	7.1	21.4	21.4	21.4	14.3	7.1	U
1	-69.928	61.98	8.87E-02	-3.45E-01	3.524	-35802.56229	1.04E-03	4.30E-04	7.1	14.3	28.6	14.3	21.4	7.1	U
2	-69.927	58.80	5.11E-02	-2.77E-01	2.507	-35802.56343	1.06E-03	4.30E-04	7.1	28.6	7.1	21.4	14.3	14.3	U
1	-69.923	60.36	1.64E-01	-2.44E-01	2.681	-35802.56314	1.07E-03	4.30E-04	7.1	14.3	21.4	28.6	14.3	7.1	U
1	-69.915	60.30	1.63E-01	-2.28E-01	0.350	-35802.56390	1.09E-03	4.20E-04	7.1	21.4	14.3	28.6	14.3	0	P
1	-69.852	58.98	1.17E-01	-2.21E-01	2.561	-35802.56331	1.11E-03	4.30E-04	0	28.6	14.3	35.7	0	7.1	U
6	-69.817	59.39	4.54E-06	-2.22E-01	1.314	-35802.56484	8.90E-04	3.90E-04	7.1	21.4	21.4	7.1	21.4	0	P
1	-69.690	63.57	2.13E-01	-2.43E-01	2.875	-35802.56295	1.19E-03	4.30E-04	7.1	21.4	14.3	21.4	21.4	0	U
1	-69.677	62.98	2.21E-01	-1.50E-01	4.054	-35802.56205	1.10E-03	4.30E-04	14.3	0	28.6	35.7	0	21.4	U
1	-69.669	61.27	2.23E-01	-1.35E-01	3.158	-35802.56299	1.10E-03	4.10E-04	14.3	7.1	21.4	35.7	0	14.3	U
2	-69.642	68.00	3.93E-02	-5.00E-01	2.705	-35802.56129	8.40E-04	4.10E-04	0	14.3	35.7	28.6	7.1	14.3	U
2	-69.604	66.15	3.33E-02	-4.72E-01	4.332	-35802.56163	9.50E-04	4.20E-04	7.1	0	50	14.3	14.3	0	U
1	-69.506	62.22	2.04E-01	-1.70E-01	4.338	-35802.56163	9.50E-04	4.20E-04	28.6	7.1	14.3	28.6	7.1	7.1	U
1	-69.400	64.61	7.54E-02	-3.65E-01	2.790	-35802.56281	1.05E-03	4.20E-04	14.3	14.3	21.4	21.4	7.1	14.3	U
1	-69.333	65.07	6.94E-02	-3.99E-01	3.530	-35802.56234	1.05E-03	4.20E-04	21.4	7.1	7.1	35.7	14.3	7.1	U
1	-68.826	56.30	7.65E-02	-1.35E-01	1.352	-35802.55989	1.39E-03	5.30E-04	7.1	0	50	21.4	14.3	0	P

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8
P U_____														

$N = 15; n = 14$

1	-74.087	55.42	7.02E-02	-1.02E-01	0.553	-38556.04637	1.26E-03	4.70E-04	0	0	60	20	13.3	0	P
4	-74.016	55.60	6.91E-02	-6.08E-02	0.926	-38556.04631	1.25E-03	4.60E-04	0	0	46.7	20	26.7	0	P
1	-73.563	59.37	1.66E-01	-2.78E-02	2.478	-38556.04483	1.36E-03	4.50E-04	6.7	0	33.3	33.3	13.3	6.7	P
2	-73.547	56.01	2.50E-03	-1.16E-01	1.233	-38556.04588	1.36E-03	4.50E-04	6.7	6.7	33.3	46.7	0	0	P
1	-73.446	57.22	5.53E-02	-5.33E-02	1.801	-38556.04540	1.15E-03	4.40E-04	0	20	20	33.3	6.7	13.3	P
1	-73.441	58.88	1.05E-01	-1.85E-01	2.383	-38556.04489	1.25E-03	4.40E-04	0	13.3	20	40	20	0	P
8	-73.440	56.06	3.08E-06	-1.17E-01	1.196	-38556.04575	1.25E-03	4.40E-04	0	0	60	6.7	26.7	0	P
2	-73.426	59.13	1.42E-01	-1.32E-01	2.150	-38556.04565	1.14E-03	4.40E-04	6.7	0	40	26.7	6.7	13.3	P
2	-73.412	59.97	1.34E-01	-1.56E-01	0.000	-38556.04501	1.25E-03	4.40E-04	6.7	0	33.3	26.7	26.7	0	P
1	-73.377	58.55	1.07E-01	-3.82E-02	2.991	-38556.04438	1.06E-03	4.30E-04	0	13.3	33.3	26.7	6.7	13.3	U
2	-73.214	59.25	1.51E-01	-1.88E-02	2.992	-38556.04436	1.33E-03	4.40E-04	6.7	6.7	46.7	20	13.3	0	U
2	-73.400	59.42	4.87E-02	-2.10E-01	2.882	-38556.04449	1.02E-03	4.30E-04	0	13.3	33.3	20	13.3	13.3	P
2	-73.097	63.54	1.27E-01	-2.56E-01	2.501	-38556.04305	1.20E-03	4.30E-04	0	26.7	20	26.7	0	13.3	P
2	-72.978	59.90	1.44E-01	-1.50E-01	2.723	-38556.04465	1.10E-04	3.00E-05	0	33.3	6.7	26.7	13.3	13.3	P
1	-72.883	65.93	8.10E-02	-3.79E-01	2.825	-38556.04258	1.10E-04	5.00E-05	0	6.7	40	26.7	6.7	6.7	P
1	-72.792	65.22	3.00E-02	-3.95E-01	4.592	-38556.04278	1.14E-03	4.20E-04	0	13.3	33.3	26.7	13.3	6.7	U
1	-72.697	61.72	1.21E-01	-2.10E-01	2.029	-38556.04473	1.37E-03	4.10E-04	6.7	33.3	6.7	33.3	6.7	6.7	P
1	-72.425	66.19	2.02E-01	-2.27E-01	3.343	-38556.04352	1.02E-03	4.00E-04	13.3	20	6.7	33.3	6.7	6.7	U
1	-72.283	67.47	1.88E-01	-2.67E-01	2.559	-38556.04281	1.20E-03	4.20E-04	20	0	33.3	13.3	20	0	P
1	-72.191	70.40	9.53E-02	-3.56E-01	5.038	-38556.04244	1.10E-03	4.00E-04	13.3	13.3	13.3	33.3	0	13.3	U
1	-72.004	70.04	6.86E-02	-4.54E-01	3.953	-38556.04140	1.09E-03	4.20E-04	13.3	0	40	13.3	13.3	13.3	U

1	-71.821	67.15	3.20E-02	-3.67E-01	2.195	-38556.04268	9.00E-04	4.00E-04	6.7	26.7	13.3	26.7	13.3	0	P
1	-71.752	65.87	2.22E-01	-1.31E-01	2.968	-38556.04415	1.01E-03	3.70E-04	13.3	20	20	6.7	13.3	6.7	P
1	-71.639	60.01	1.16E-01	-1.57E-01	2.371	-38556.04065	1.52E-03	5.30E-04	0	33.3	20	13.3	20	6.7	P
2	-73.337	60.87	2.73E-02	-2.03E-01	3.366	-38556.04378	1.00E-03	4.40E-04	0	13.3	46.7	13.3	0	0	U
2	-73.323	60.85	7.62E-02	-2.77E-01	2.950	-38556.04445	1.42E-03	4.30E-04	6.7	0	26.7	40	20	0	P
2	-73.283	57.52	6.97E-02	-1.77E-01	1.218	-38556.04497	1.33E-03	4.40E-04	6.7	6.7	46.7	20	13.3	0	P
1	-73.165	60.78	1.35E-01	-1.05E-01	3.293	-38556.04389	1.00E-03	4.30E-04	0	26.7	26.7	20	0	13.3	U
2	-73.152	59.58	8.65E-03	-1.78E-01	2.277	-38556.04511	1.07E-03	4.30E-04	0	20	20	40	0	0	P
2	-73.094	58.87	4.28E-02	-4.20E-03	2.872	-38556.04438	1.22E-03	4.40E-04	0	40	13.3	6.7	13.3	13.3	P
1	-73.046	60.33	1.77E-01	-1.05E-01	2.924	-38556.04409	1.01E-03	4.20E-04	0	20	13.3	40	6.7	0	P
2	-73.032	59.04	1.24E-01	-8.91E-03	2.807	-38556.04439	1.17E-03	4.30E-04	6.7	13.3	33.3	20	0	6.7	P
1	-72.956	62.55	2.34E-01	-7.97E-02	3.855	-38556.04357	1.20E-03	4.20E-04	6.7	6.7	26.7	33.3	13.3	6.7	U
1	-72.918	63.02	1.66E-01	-2.33E-01	3.095	-38556.04411	1.17E-03	4.20E-04	0	20	26.7	26.7	6.7	6.7	U
2	-72.860	61.76	4.19E-02	-1.64E-01	3.387	-38556.04390	9.70E-04	4.20E-04	6.7	20	26.7	20	0	0	U
1	-72.858	62.45	2.06E-01	-9.07E-02	1.817	-38556.04320	1.21E-03	4.30E-04	6.7	13.3	33.3	20	0	6.7	P
1	-72.828	64.54	1.77E-01	-2.32E-01	3.981	-38556.04337	1.16E-03	4.30E-04	0	26.7	20	20	6.7	20	U
1	-72.791	63.11	1.24E-01	-2.37E-01	2.875	-38556.04431	1.38E-03	4.30E-04	0	26.7	20	20	20	0	P
1	-72.786	63.61	1.65E-01	-1.92E-01	3.240	-38556.04405	1.08E-03	4.10E-04	6.7	20	20	20	6.7	13.3	U
1	-72.727	61.41	1.47E-01	-1.50E-01	4.111	-38556.04336	1.14E-03	4.20E-04	6.7	20	13.3	26.7	20	6.7	U
1	-72.720	61.69	1.14E-01	-1.02E-01	3.997	-38556.04335	1.10E-03	4.30E-04	13.3	20	20	6.7	13.3	13.3	U
2	-72.685	68.57	1.53E-01	-3.69E-01	3.555	-38556.04381	8.10E-04	4.10E-04	0	26.7	20	20	13.3	0	U

2	-72.664	63.39	2.50E-01	-1.27E-01	3.528	-38556.04387	1.02E-03	4.20E-04	0	26.7	26.7	20	13.3	0	U
2	-72.649	63.56	1.63E-01	-1.91E-01	4.093	-38556.04309	1.22E-03	4.30E-04	13.3	0	53.3	6.7	0	13.3	U
1	-72.648	61.05	3.88E-02	-1.82E-01	3.959	-38556.04347	9.80E-04	4.20E-04	6.7	13.3	26.7	26.7	6.7	13.3	U
2	-72.638	65.89	1.08E-01	-3.49E-01	4.467	-38556.04304	9.30E-04	4.10E-04	6.7	0	26.7	46.7	13.3	0	U
1	-72.610	61.65	1.31E-01	-7.36E-02	3.550	-38556.04350	1.22E-03	4.30E-04	6.7	20	13.3	33.3	6.7	13.3	U
1	-72.604	64.19	1.49E-01	-1.97E-01	3.618	-38556.04395	1.14E-03	3.90E-04	6.7	20	13.3	33.3	6.7	13.3	U
2	-72.399	64.64	6.24E-02	-3.19E-01	5.123	-38556.04224	1.04E-03	4.20E-04	0	26.7	20	33.3	0	0	U
1	-72.388	63.03	9.14E-02	-1.67E-01	3.428	-38556.04295	1.27E-03	4.30E-04	13.3	13.3	26.7	20	0	6.7	U
1	-72.354	65.95	9.96E-02	-3.31E-01	4.270	-38556.04328	1.08E-03	3.90E-04	6.7	20	13.3	33.3	6.7	13.3	U
2	-72.330	57.15	4.49E-02	-1.74E-01	1.442	-38556.04290	1.22E-03	5.40E-04	6.7	13.3	40	26.7	6.7	0	P

Sym.	E_{PES}	ρ^2	ξ^+	ξ^-	ΔE_{DFT}^{Opt}	E_{DFT}^{SP}	Gmax	Grms	CN_3	CN_4	CN_5	CN_6	CN_7	CN_8	P U
$N = 17; n = 16$															
6	-79.833	65.30	1.43E-06	-3.04E-01	0.367	-44063.00580	1.19E-03	4.00E-04	0	0	17.6	58.8	0	0	P
4	-79.575	62.89	2.19E-02	-1.73E-01	1.101	-44063.00644	1.60E-03	4.40E-04	0	11.8	5.9	41.2	35.3	0	P
2	-79.560	62.02	6.17E-02	-8.49E-02	0.571	-44063.00693	1.46E-03	4.40E-04	0	11.8	17.6	29.4	23.5	11.8	P
2	-79.536	62.98	2.36E-02	-1.73E-01	0.599	-44063.00683	1.18E-03	4.40E-04	0	11.8	5.9	52.9	11.8	11.8	P
4	-79.518	62.11	6.17E-02	-8.93E-02	0.119	-44063.00735	1.35E-03	4.50E-04	0	11.8	17.6	41.2	0	23.5	P
1	-79.470	61.95	3.45E-02	-4.39E-02	0.805	-44063.00652	6.20E-04	1.00E-04	0	23.5	17.6	23.5	23.5	5.9	P
2	-79.350	62.85	5.01E-02	-7.14E-02	0.888	-44063.00644	5.00E-04	8.00E-05	0	11.8	29.4	29.4	23.5	0	P

2	-79.344	62.55	1.61E-02	-1.21E-02	0.814	-44063.00654	1.06E-03	4.30E-04	0	11.8	23.5	29.4	17.6	11.8	P
2	-79.306	63.38	2.38E-02	-1.80E-01	0.069	-44063.00745	1.20E-03	4.20E-04	0	5.9	29.4	35.3	11.8	0	P
1	-79.297	62.13	9.37E-02	-6.94E-02	0.771	-44063.00662	1.42E-03	1.60E-04	5.9	5.9	29.4	29.4	11.8	11.8	P
2	-79.180	65.87	6.98E-02	-1.55E-01	1.987	-44063.00560	1.32E-03	4.20E-04	0	11.8	29.4	35.3	0	0	U
2	-79.052	61.24	2.72E-02	-3.16E-02	1.460	-44063.00602	6.50E-04	1.30E-04	0	11.8	41.2	17.6	23.5	0	P
1	-78.917	67.17	1.44E-01	-1.61E-01	2.860	-44063.00478	1.55E-03	4.20E-04	0	11.8	29.4	23.5	17.6	11.8	U
2	-78.880	64.32	8.55E-02	-6.00E-02	0.792	-44063.00518	1.55E-03	4.20E-04	0	17.6	17.6	29.4	17.6	11.8	P
1	-78.779	64.82	7.00E-02	-7.49E-02	2.860	-44063.00478	1.36E-03	4.30E-04	0	23.5	29.4	17.6	5.9	11.8	U
2	-78.696	65.83	9.99E-03	-1.07E-01	2.706	-44063.00446	4.44E-03	2.60E-04	0	23.5	35.3	11.8	0	5.9	U
2	-78.696	67.85	9.37E-02	-1.46E-01	1.004	-44063.00446	1.27E-03	4.30E-04	0	23.5	35.3	11.8	0	5.9	P
1	-78.447	68.83	1.31E-01	-1.46E-01	3.021	-44063.00463	1.56E-03	4.20E-04	5.9	11.8	17.6	35.3	5.9	11.8	U
2	-78.385	71.73	7.50E-02	-3.53E-01	2.308	-44063.00540	1.26E-03	4.10E-04	0	11.8	29.4	23.5	17.6	11.8	U
1	-78.273	70.13	1.54E-01	-2.50E-01	1.362	-44063.00456	1.08E-03	4.00E-04	0	17.6	35.3	17.6	11.8	0	P
1	-78.190	68.27	8.87E-02	-2.95E-01	1.992	-44063.00422	6.60E-04	1.10E-04	5.9	5.9	17.6	41.2	23.5	0	U
1	-78.003	68.20	1.96E-01	-8.03E-02	3.045	-44063.00461	1.09E-03	4.10E-04	5.9	11.8	29.4	23.5	5.9	11.8	U
1	-77.968	69.39	1.25E-01	-2.42E-01	4.442	-44063.00326	7.00E-04	1.00E-04	5.9	17.6	11.8	35.3	11.8	11.8	U
1	-77.800	76.36	4.56E-02	-4.29E-01	0.309	-44063.00457	1.35E-03	3.90E-04	5.9	5.9	35.3	23.5	5.9	17.6	P
1	-76.795	74.38	1.18E-01	-1.93E-01	4.424	-44063.00313	1.19E-03	3.70E-04	17.6	17.6	11.8	17.6	5.9	17.6	U
1	-79.230	64.85	1.09E-01	-1.55E-01	0.822	-44063.00313	1.20E-03	1.00E-04	0	11.8	29.4	35.3	11.8	0	P
1	-79.161	65.02	1.10E-01	-1.03E-01	1.612	-44063.00593	1.37E-03	4.40E-04	5.9	5.9	11.8	41.2	23.5	5.9	P
1	-78.917	64.25	4.88E-02	-9.56E-02	1.348	-44063.00619	1.13E-03	4.50E-04	5.9	5.9	23.5	23.5	23.5	11.8	P

4	-78.857	66.16	1.37E-02	-3.20E-01	1.834	-44063.00561	1.25E-03	4.50E-04	0	35.3	17.6	17.6	11.8	11.8	U
1	-78.774	64.89	8.82E-03	-9.71E-02	2.498	-44063.00528	1.07E-03	4.10E-04	0	17.6	17.6	41.2	5.9	0	U
1	-78.710	69.03	1.04E-01	-2.77E-01	3.400	-44063.00427	1.20E-03	4.10E-04	0	11.8	17.6	35.3	17.6	11.8	U
1	-78.679	68.39	1.09E-01	-2.37E-01	2.468	-44063.00513	1.47E-03	4.20E-04	5.9	0	41.2	29.4	0	11.8	U
1	-78.673	66.44	8.35E-02	-1.48E-01	0.233	-44063.00429	1.49E-03	1.30E-04	17.6	11.8	23.5	11.8	11.8	0	P
1	-78.658	66.04	6.62E-02	-2.66E-01	1.265	-44063.00475	6.10E-04	9.00E-05	0	5.9	41.2	23.5	17.6	5.9	P
1	-78.632	66.22	1.01E-01	-1.32E-01	3.163	-44063.00452	1.11E-03	4.20E-04	5.9	5.9	35.3	23.5	0	11.8	U
1	-78.625	66.28	1.07E-01	-1.42E-01	1.517	-44063.00582	1.53E-03	4.30E-04	11.8	0	35.3	11.8	17.6	17.6	P
1	-78.531	67.78	8.32E-02	-2.21E-01	2.429	-44063.00514	1.57E-03	4.40E-04	11.8	0	23.5	23.5	29.4	5.9	U
1	-78.527	68.91	1.77E-01	-1.31E-01	1.265	-44063.00517	1.53E-03	4.10E-04	5.9	11.8	23.5	23.5	11.8	11.8	P
1	-78.502	65.04	1.73E-02	-3.36E-02	3.071	-44063.00449	1.17E-03	4.10E-04	5.9	11.8	35.3	23.5	0	0	U
2	-78.439	67.76	1.44E-01	-2.18E-01	2.948	-44063.00497	1.23E-03	4.20E-04	0	35.3	0	52.9	0	0	U
2	-78.403	70.25	8.08E-02	-3.31E-01	2.058	-44063.00558	9.70E-04	4.10E-04	0	11.8	35.3	23.5	11.8	0	U
2	-78.356	69.63	3.98E-02	-2.54E-01	3.508	-44063.00405	2.00E-05	1.00E-05	5.9	17.6	35.3	5.9	5.9	5.9	U
1	-78.250	71.13	9.54E-02	-3.02E-01	1.198	-44063.00420	1.20E-03	4.10E-04	5.9	11.8	17.6	17.6	35.3	5.9	P
1	-78.219	70.09	1.69E-01	-2.15E-01	2.978	-44063.00327	1.24E-03	4.00E-04	0	17.6	29.4	17.6	17.6	5.9	U
1	-78.207	69.46	1.21E-01	-2.53E-01	1.128	-44063.00432	1.46E-03	4.30E-04	5.9	11.8	17.6	23.5	35.3	0	P
1	-78.166	70.66	1.94E-01	-1.63E-01	1.168	-44063.00309	1.16E-03	4.00E-04	0	29.4	23.5	11.8	5.9	11.8	P
1	-78.122	72.27	8.21E-02	-3.56E-01	0.428	-44063.00310	1.13E-03	4.00E-04	11.8	17.6	17.6	17.6	11.8	5.9	P
2	-78.119	72.03	1.10E-02	-3.73E-01	3.448	-44063.00434	1.17E-03	3.80E-04	5.9	5.9	35.3	11.8	11.8	23.5	U
1	-78.119	71.84	6.26E-02	-3.66E-01	3.997	-44063.00371	1.59E-03	4.20E-04	5.9	0	35.3	23.5	23.5	0	U

1	-78.107	69.58	1.56E-01	-2.12E-01	3.333	-44063.00401	1.22E-03	4.10E-04	0	23.5	17.6	29.4	5.9	5.9	U
2	-78.002	70.07	4.69E-03	-3.55E-01	4.812	-44063.00287	1.16E-03	4.00E-04	0	17.6	23.5	35.3	5.9	0	U
1	-77.922	72.09	1.97E-01	-1.80E-01	3.723	-44063.00340	1.33E-03	4.00E-04	5.9	17.6	35.3	5.9	11.8	11.8	U
2	-77.920	66.07	3.26E-02	-2.86E-01	0.000	-44063.00083	6.40E-04	1.30E-04	0	17.6	5.9	47.1	11.8	5.9	P
1	-77.909	68.74	9.51E-02	-1.76E-01	4.587	-44063.00319	1.16E-03	4.10E-04	0	35.3	17.6	11.8	5.9	23.5	U