Anexo 1

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1 Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees.

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
HF		-1247.69	-1247.77	-1248.07	-1246.88	-1247.18	-1247.45	387.01	45.29
HF	6-31g	-1261.29	-1261.36	-1261.49	-1260.13	-1260.25	-1260.44	654.70	7.45
HF	6-31g(d,p)	-1261.30	-1261.36	-1261.49	-1260.14	-1260.25	-1260.44	655.82	7.29
HF	6-31+g	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	657.64	7.04
HF	6-31+g(d,p)	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	658.73	6.88
HF	6-31++g	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	657.64	7.04
HF	6-31++g(d,p)	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	658.73	6.88
HF	cc-pVDZ	-1261.47	-1261.50	-1261.66	-1260.30	-1260.42	-1260.61	661.75	6.46
HF	cc-pVTZ	-1261.48	-1261.54	-1261.66	-1260.31	-1260.43	-1260.62	657.96	6.99
HF	cc-pVQZ	-1261.48	-1261.54	-1261.67	-1260.32	-1260.43	-1260.62	658.33	6.94
HF	AUG-cc-pVDZ	-1261.47	-1261.50	-1261.66	-1260.31	-1260.42	-1260.61	661.56	6.48
HF	AUG-cc-pVTZ	-1261.48	-1261.54	-1261.66	-1260.31	-1260.43	-1260.62	658.00	6.99
HF	AUG-cc-pVQZ	-1261.48	-1261.54	-1261.67	-1260.32	-1260.39	-1260.62	658.33	6.94
HF	SV	-1261.28	-1261.34	-1261.47	-1260.10	-1260.22	-1260.41	664.79	6.03
HF	SVP	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
HF	TZV	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.51	7.34
HF	TZVP	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.46	7.35
HF	QZVP	-1261.48	-1261.54	-1261.67	-1260.31	-1260.39	-1260.62	658.18	6.96
HF	def2SV	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
HF	def2SVP	-1261.29	-1261.35	-1261.48	-1260.11	-1260.23	-1260.42	663.98	6.14
HF	def2SVPP	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
HF	def2TZV	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.51	7.34
HF	def2TZVP	-1261.45	-1261.51	-1261.64	-1260.29	-1260.40	-1260.59	657.15	7.11
HF	def2TZVPP	-1261.45	-1261.47	-1261.64	-1260.29	-1260.40	-1260.59	657.85	7.01
HF	def2QZV	-1261.47	-1261.53	-1261.66	-1260.30	-1260.42	-1260.62	655.28	7.37
HF	def2QZVP	-1261.48	-1261.50	-1261.67	-1260.31	-1260.43	-1260.62	658.18	6.96
HF	def2QZVPP	-1261.48	-1261.50	-1261.67	-1260.32	-1260.39	-1260.62	658.29	6.95
B3LYP		-1248.85	-1249.04	-1249.15	-1248.02	-1248.14	-1248.26	563.39	20.36
B3LYP	6-31g	-1262.50	-1262.55	-1262.64	-1261.26	-1261.35	-1261.49	721.55	2.00
B3LYP	6-31g(d,p)	-1262.50	-1262.55	-1262.64	-1261.26	-1261.35	-1261.49	721.86	2.04
B3LYP	6-31+g	-1262.52	-1262.57	-1262.66	-1261.27	-1261.36	-1261.50	728.83	3.03

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
B3LYP	6-31+g(d,p)	-1262.52	-1262.57	-1262.66	-1261.27	-1261.36	-1261.50	729.13	3.07
B3LYP	6-31++g	-1262.52	-1262.57	-1262.66	-1261.27	-1261.36	-1261.50	728.83	3.03
B3LYP	6-31++g(d,p)	-1262.52	-1262.57	-1262.66	-1261.27	-1261.36	-1261.50	729.13	3.07
B3LYP	cc-pVDZ	-1262.68	-1262.73	-1262.82	-1261.43	-1261.52	-1261.66	729.53	3.13
B3LYP	cc-pVTZ	-1262.68	-1262.73	-1262.83	-1261.43	-1261.53	-1261.67	728.12	2.93
B3LYP	cc-pV1Z	-1262.69	-1262.74	-1262.83	-1261.44	-1261.53	-1261.67	728.46	2.97
B3LYP	AUG-cc-pVDZ	-1262.68	-1262.73	-1262.82	-1261.43	-1261.52	-1261.66	729.42	3.11
B3LYP	AUG-cc-pVTZ	-1262.68	-1262.70	-1262.83	-1261.43	-1261.53	-1261.67	728.13	2.93
B3LYP	AUG-cc-pVQZ	-1262.69	-1262.74	-1262.83	-1261.44	-1261.49	-1261.67	728.46	2.97
B3LYP	SV SV	-1262.49	-1262.74	-1262.63	-1261.22	-1261.32	-1261.46	736.56	4.12
B3LYP	SVP	-1262.49	-1262.54	-1262.63	-1261.23	-1261.32	-1261.46	734.54	3.83
B3LYP	TZV	-1262.65	-1262.71	-1262.80	-1261.41	-1261.50	-1261.64	726.33	2.67
B3LYP	TZVP	-1262.65	-1262.71	-1262.80	-1261.41	-1261.50	-1261.64	726.54	2.70
B3LYP	QZVP	-1262.68	-1262.71	-1262.83	-1261.41	-1261.53	-1261.67	728.47	2.70
B3LYP	def2SV	-1262.49	-1262.74	-1262.63	-1261.43	-1261.33	-1261.46	734.54	3.83
B3LYP	def2SVP	-1262.49	-1262.54	-1262.63	-1261.23	-1261.32	-1261.46	735.18	3.92
B3LYP	def2SVPP def2TZV	-1262.49	-1262.54	-1262.63	-1261.23	-1261.32	-1261.46	734.54	3.83
B3LYP		-1262.65	-1262.71	-1262.80	-1261.41	-1261.50	-1261.64	726.33	2.67
B3LYP	def2TZVP	-1262.65	-1262.71	-1262.80	-1261.41	-1261.50	-1261.64	726.95	2.76
B3LYP	def2TZVPP	-1262.65	-1262.71	-1262.80	-1261.41	-1261.46	-1261.64	727.44	2.83
B3LYP	def2QZV	-1262.68	-1262.73	-1262.83	-1261.43	-1261.53	-1261.67	727.30	2.81
B3LYP	def2QZVP	-1262.68	-1262.74	-1262.83	-1261.43	-1261.53	-1261.67	728.47	2.98
B3LYP	def2QZVPP	-1262.68	-1262.74	-1262.83	-1261.43	-1261.53	-1261.67	728.56	2.99
B3P86		-1249.38	-1249.58	-1249.69	-1248.55	-1248.62	-1248.79	565.00	20.13
B3P86	6-31g	-1263.01	-1263.06	-1263.16	-1261.75	-1261.84	-1261.99	735.21	3.93
B3P86	6-31g(d,p)	-1263.01	-1263.06	-1263.16	-1261.75	-1261.84	-1261.99	735.54	3.98
B3P86	6-31+g	-1263.02	-1263.08	-1263.17	-1261.75	-1261.85	-1261.99	741.16	4.77
B3P86	6-31+g(d,p)	-1263.02	-1263.08	-1263.17	-1261.75	-1261.85	-1261.99	741.48	4.81
B3P86	6-31++g	-1263.02	-1263.08	-1263.17	-1261.75	-1261.85	-1261.99	741.16	4.77
B3P86	6-31++g(d,p)	-1263.02	-1263.08	-1263.17	-1261.75	-1261.85	-1261.99	741.48	4.81
B3P86	cc-pVDZ	-1263.18	-1263.24	-1263.34	-1261.92	-1262.01	-1262.15	741.47	4.81
B3P86	cc-pVTZ	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	739.55	4.54
B3P86	cc-pVQZ	-1263.19	-1263.25	-1263.34	-1261.93	-1262.02	-1262.16	740.06	4.61
B3P86	AUG-cc-pVDZ	-1263.18	-1263.24	-1263.34	-1261.92	-1262.01	-1262.15	741.34	4.79
B3P86	AUG-cc-pVTZ	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	739.56	4.54
B3P86	AUG-cc-pVQZ	-1263.19	-1263.25	-1263.34	-1261.93	-1262.02	-1262.16	740.05	4.61
B3P86	SV	-1262.99	-1263.05	-1263.15	-1261.71	-1261.81	-1261.95	748.46	5.80
B3P86	SVP	-1263.00	-1263.01	-1263.15	-1261.72	-1261.77	-1261.96	746.11	5.47
B3P86	TZV	-1263.16	-1263.21	-1263.31	-1261.89	-1261.99	-1262.13	737.78	4.29
B3P86	TZVP	-1263.16	-1263.21	-1263.31	-1261.89	-1261.99	-1262.13	737.92	4.31
B3P86	QZVP	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	739.89	4.59
B3P86	def2SV	-1263.00	-1263.05	-1263.15	-1261.72	-1261.81	-1261.96	746.11	5.47
B3P86	def2SVP	-1263.00	-1263.05	-1263.15	-1261.72	-1261.81	-1261.96	746.77	5.56
B3P86	def2SVPP	-1263.00	-1263.05	-1263.15	-1261.72	-1261.81	-1261.96	746.11	5.47
B3P86	def2TZV	-1263.16	-1263.21	-1263.31	-1261.89	-1261.99	-1262.13	737.78	4.29
B3P86	def2TZVP	-1263.16	-1263.21	-1263.31	-1261.89	-1261.99	-1262.13	738.35	4.37
B3P86	def2TZVPP	-1263.16	-1263.22	-1263.31	-1261.90	-1261.99	-1262.13	738.81	4.44
B3P86	def2QZV	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	738.66	4.42
B3P86	def2QZVP	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	739.89	4.59
B3P86	def2QZVPP	-1263.19	-1263.24	-1263.34	-1261.92	-1262.02	-1262.16	739.98	4.60
O3LYP		-1241.66	-1249.25	-1249.39	-1248.22	-1248.31	-1248.49	561.28	20.66

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

OSIYP (OSIY) 6-31g(h) 1-1922.65 1-1262.70 1-202.82 1-214.24 1-216.16 -161.65 1.33 OSIYP (OSIY) 6-31 (H) 1-1262.67 1-262.72 1-262.82 1-216.15 1-261.66 1-261.68 733.37 2.24 OSIYP (OSIY) 6-31 (H) 1-262.67 1-262.72 1-262.83 1-261.45 1-261.66 1-261.68 733.37 2.24 OSIYP (OSIY) 6-31 (H) 1-262.67 1-262.72 1-262.83 1-261.45 1-261.56 1-261.68 723.27 2.24 OSIYP (OSIY) 1-262.67 1-262.72 1-262.83 1-261.45 1-261.56 1-261.68 723.57 2.28 OSIYP (OSIY) 1-262.83 1-262.88 1-263.00 1261.62 1-261.85 723.45 2.26 OSIYP (OSIY) 1-262.83 1-262.88 1-263.00 1-261.62 1-261.81 723.45 2.23 OSIYP (OSIY) 1-262.83 1-262.88 1-263.00 1-261.69 1-261.84 725.18 723.34 2.22	Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
O3I/P (O3I/P) 6-31+g(d,p) 1262.67 -1262.72 -1262.83 -1261.45 -1261.56 -1261.68 723.27 2.24 O3I/P (O3I/P) 6-31+rg -1262.72 -1262.82 -1262.83 -1261.45 -1261.56 -1261.68 723.57 2.24 O3I/P (O3I/P) 6-31+rg(d,p) -1262.87 -1262.83 -1261.45 -1261.56 -1261.68 723.57 2.24 O3I/P (O5PVIZ) -1262.83 -1263.00 -1261.69 -1261.72 -1261.84 725.41 2.54 O3I/P (O5PVIZ) -1262.83 -1263.00 -1261.62 -1261.73 -1261.85 723.40 2.26 O3I/P (O5PVIZ) -1262.83 -1262.89 -1263.00 -1261.62 -1261.73 -1261.84 725.32 2.23 O3I/P (O5PVIZ) -1262.83 -1262.89 -1263.00 -1261.62 -1261.73 -1261.84 725.34 2.23 O3I/P (O5PVIZ) -1262.83 -1262.89 -1263.00 -1261.62 -1261.73 -1261.85 723.43 2.23 <	O3LYP		-1262.65	-1262.70	-1262.82	-1261.42	-1261.56	-1261.67		1.26
OSIAP G-31+g(d,p) 1262.67 -1262.72 -1262.83 -1261.45 -1261.66 -1261.68 723.55 2.28	O3LYP	6-31g(d,p)	-1262.65	-1262.70	-1262.82	-1261.42	-1261.56	-1261.67	716.65	1.30
OSIAP G-31+g(d,p) 1262.67 -1262.72 -1262.83 -1261.45 -1261.66 -1261.68 723.55 2.28	O3LYP	6-31+g	-1262.67	-1262.72	-1262.83	-1261.45	-1261.56	-1261.68	723.27	2.24
OSIYP 6-31+++g(d,p) -1262.67 -1262.72 -1262.83 -1261.45 -1261.56 -1261.68 723.57 2.24 OSIYP ccpVDZ -1262.83 -1262.83 -1262.83 -1262.84 -1263.95 -1261.84 -1261.84 725.41 2.26 OSIYP ccpVQZ -1262.84 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 723.40 2.26 OSIYP AUG-ccpVQZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 723.59 2.29 OSIYP AUG-ccpVZ -1262.83 -1262.89 -1263.00 -1261.62 -1261.73 -1261.85 723.59 2.29 OSIYP AUG-ccpVZ -1262.81 -1262.81 -1261.62 -1261.73 -1261.85 723.53 2.23 OSIYP AUG-ccpVZ -1262.84 -1262.89 -1261.80 -1261.83 -1261.53 -1261.63 -1261.63 -1261.63 -1261.63 -1261.64 -730.88 -2.32 OSIYP <t< td=""><td>O3LYP</td><td></td><td></td><td>-1262.72</td><td>-1262.83</td><td>-1261.45</td><td>-1261.56</td><td>-1261.68</td><td>723.55</td><td></td></t<>	O3LYP			-1262.72	-1262.83	-1261.45	-1261.56	-1261.68	723.55	
OSIVP (A) 6-31++g(d,p) -1262.67 -1262.72 -1262.83 -1261.45 -1261.72 -1261.84 -23.55 2.28 OSIVP (C) ccpVVZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.73 -1261.84 725.41 2.54 OSIVP (C) ccpVVZ -1262.84 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 723.59 2.29 OSIVP (C) AUG-ccpVVZ -1262.84 -1262.88 -1263.00 -1261.62 -1261.73 -1261.87 723.59 2.29 OSIVP (A) AUG-ccpVVZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.87 7261.85 723.34 2.26 OSIVP (A) AUG-ccpVVZ -1262.44 -1262.90 -1262.81 -1261.62 -1261.73 -1261.85 723.43 2.26 OSIVP (SVP) -1262.64 -1262.69 -1262.81 -1261.80 -1261.81 7261.82 721.93 2.27 OSIVP (C) -1262.81 -1262.86 -1262.97 -1261.59	O3LYP	6-31++g			-1262.83	-1261.45		-1261.68		
OSIYP cc-pVDZ -1262.88 -1262.88 -1263.00 -1261.69 -1261.73 -1261.84 725.40 22.64 OSIYP cc-pVQZ -1262.84 -1262.89 -1263.00 -1261.62 -1261.73 -1261.85 723.59 2.29 OSIYP AUG-cc-pVZ -1262.83 -1262.89 -1263.00 -1261.62 -1261.73 -1261.85 723.39 2.29 OSIYP AUG-cc-pVZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 723.32 2.53 OSIYP AUG-cc-pVZ -1262.84 -1262.89 -1263.00 -1261.62 -1261.73 -1261.85 723.85 2.26 OSIYP AUG-cc-pVZ -1262.44 -1262.96 -1262.81 -1261.59 -1261.62 -1261.63 732.85 2.32 OSIYP SV -1262.64 -1262.96 -1262.81 -1261.59 -1261.70 -1261.83 722.17 2.161.83 722.17 -1261.82 722.17 2.161.82 722.17 2.161.83 <		6-31++g(d,p)		-1262.72	-1262.83			-1261.68		
OSIYP cc-pVTZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 723.40 2.29 OSIYP AUG-cc-pVTZ -1262.83 -1263.00 -1261.69 -1261.72 -1261.85 723.59 2.29 OSIYP AUG-cc-pVTZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.72 -1261.85 723.43 2.26 OSIYP AUG-cc-pVTZ -1262.48 -1262.99 -1263.00 -1261.62 -1261.73 -1261.85 723.43 2.26 OSIYP AUG-cc-pVTZ -1262.48 -1262.99 -1262.81 -1261.52 -1261.64 732.78 3.59 OSIYP SVP -1262.44 -1262.69 -1262.81 -1261.59 -1261.64 732.78 3.59 OSIYP TZV -1262.81 -1262.86 -1262.97 -1261.59 -1261.64 730.48 3.26 OSIYP -1262.81 -1262.89 -1262.81 -1262.82 -1261.62 730.17 3.22 OSIYP		cc-pVDZ								
OSIVP ccpVQZ 1262.84 1-1262.89 1-263.00 -1261.62 1261.73 -1261.85 723.59 2.29 OSIVP AUG-ccpVDZ -1262.83 -1262.88 -1263.00 -1261.62 -1261.73 -1261.85 733.43 2.26 OSIVP AUG-ccpVQZ -1262.83 -1262.69 -1263.00 -1261.62 -1261.85 723.43 2.26 OSIVP SV -1262.64 -1262.69 -1262.81 -1261.03 1261.62 -1261.85 733.85 2.32 OSIVP SVP -1262.64 -1262.69 -1262.81 -1261.38 1261.52 -1261.64 730.48 3.26 OSIVP TZV -1262.81 -1262.86 -1262.97 -1261.38 -1261.82 722.17 2.08 OSIVP TZVP -1262.81 -1262.66 -1262.81 -1261.59 -1261.82 722.17 2.08 OSIVP def2SVP -1262.81 -1263.99 -1262.81 -1261.59 -1261.62 -1261.87 -1261.67 -1										
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APFD def2TZVPP -1262.48 -1262.53 -1262.64 -1261.25 -1261.31 -1261.49 720.93 1.91										1.75
					-1262.64		-1261.39		720.45	1.84
APFD def2QZV -1262.51 -1262.56 -1262.67 -1261.28 -1261.41 -1261.52 720.46 1.84	APFD	def2TZVPP	-1262.48	-1262.53	-1262.64	-1261.25	-1261.31	-1261.49	720.93	1.91
	APFD	def2QZV	-1262.51	-1262.56	-1262.67	-1261.28	-1261.41	-1261.52	720.46	1.84

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

APFD def2QZVP - 1262.51 - 1262.56 - 1262.67 - 1261.28 - 1261.42 - 1261.52 - 721.76 - 2.03 APFD def2QZVPP - 1262.51 - 1262.56 - 1262.67 - 1261.88 - 1261.52 - 1261.52 - 721.76 - 2.03 wB97KD - 1248.76 - 1248.78 - 1248.98 - 1249.19 - 1248.69 - 1248.17 - 1248.33 - 1251.55 - 2.04 wB97KD - 6.31g (-) - 1262.31 - 1262.35 - 1262.65 - 1262.31 - 1261.33 - 1261.51 - 715.50 - 1.14 wB97KD - 6.31g (d.p) - 1262.32 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 712.97 - 2.06 wB97KD - 6.31-g (d.p) - 1262.52 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 721.97 - 2.06 wB97KD - 6.31-g (d.p) - 1262.52 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 721.97 - 2.06 wB97KD - 6.31-g (d.p) - 1262.52 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 721.97 - 2.06 wB97KD - 6.31-g (d.p) - 1262.52 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 721.97 - 2.06 wB97KD - 6.31-g (d.p) - 1262.50 - 1262.60 - 1262.66 - 1261.30 - 1261.33 - 1261.51 - 721.97 - 2.06 wB97KD - c-pVTZ - 1262.50 - 1262.64 - 1262.65 - 1262.68 - 1261.80 - 1261.54 - 1261.68 - 717.67 - 1.45 wB97KD - c-pVTZ - 1262.50 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.68 - 718.67 - 1.46 wB97KD - AUG-c-pVTZ - 1262.51 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.63 - 1.59 wB97KD - AUG-c-pVTZ - 1262.51 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.53 - 1.59 wB97KD - AUG-c-pVTZ - 1262.51 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.53 - 1.59 wB97KD - AUG-c-pVTZ - 1262.51 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.15 - 1.50 wB97KD - SVP - 1262.50 - 1262.64 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.15 - 1.66 wB97KD - SVP - 1262.50 - 1262.65 - 1262.83 - 1261.49 - 1261.55 - 1261.69 - 718.15 - 1.66 wB97KD - 3262.50 - 1262.65 - 1262.54 - 1262.65 - 1261.33 - 1261.48 - 723.15 - 222.8 wB97KD - 3262.50 - 1262.64 - 1262.65 - 1262.65 - 1262.65 - 1262.65 - 1262.65 - 1261.30 - 1261.48 - 723.15 - 222.60 - 1262.65 - 1262.65 - 1262.65 - 1262.65 - 1261.30 - 1261.68 - 7163.40 - 7163.40 - 7262.80 - 7262.80 - 7262.80 - 7262.80 - 7262.80 - 72	Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
WB9TXD -1248.76 -1248.98 -1249.19 -1248.10 -1248.33 542.88 23.26 WB9TXD 6-31g(d.p) -1262.31 -1262.46 -1262.65 -1261.31 -1261.37 -1261.51 715.50 1.19 WB9TXD 6-31g(d.p) -1262.32 -1262.60 -1262.65 -1261.30 -1261.33 -1261.51 712.97 2.06 WB9TXD 6-31g(d.p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.57 722.29 2.10 WB9TXD 6-31g(d.p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.57 722.79 2.06 WB9TXD 6-31g(d.p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.64 7261.63 -1261.64 1261.68 719.84 1.76 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 4.06 <td>APFD</td> <td>def2QZVP</td> <td>-1262.51</td> <td>-1262.56</td> <td>-1262.67</td> <td>-1261.28</td> <td>-1261.42</td> <td>-1261.52</td> <td></td> <td>2.03</td>	APFD	def2QZVP	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52		2.03
wB97XD 6-31g (Ap) 1292.31 1292.46 -1292.65 -1261.31 -1261.31 -1261.33 -1261.51 715.85 114 wB97XD 6-31+g (Ap) 1292.31 -1262.60 -1262.60 -1261.30 -1261.33 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g (Ap) 1262.52 -1262.60 -1262.60 -1262.60 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g (Ap) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g (Ap) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g (Ap) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g (Ap) -1262.51 -1262.52 -1262.65 -1262.83 -1261.48 -1261.54 -1261.65 71261.67 722.99 2.10 wB97XD c-pVDZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.54 -1261.68 7167.67 1.45 wB97XD AUG-ce-pVDZ -1262.51 -1262.64 -1262.83 -1261.49 -1261.55 -1261.68 7163.75 7166.69 716.63 1.55 wB97XD AUG-ce-pVDZ -1262.51 -1262.64 -1262.60 -1262.70 -1261.49 -1261.65 -1261.68 7163.70 719.15 1.66 wB97XD AUG-ce-pVDZ -1262.51 -1262.64 -1262.60 -1262.70 -1262.80 -1261.49 -1261.55 -1261.68 7163.70 719.15 1.66 wB97XD AUG-ce-p	APFD	def2QZVPP	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	721.85	2.04
wB97XD 6-31g 1-1923.31 1-262.46 -1262.65 -1261.31 -1261.33 -1261.51 715.85 1.14 wB97XD 6-31g(d.p) -1262.31 1-262.60 -1261.30 -1261.33 -1261.51 721.77 2.06 wB97XD 6-31+g(d.p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.77 2.06 wB97XD 6-31++g(d.p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 722.29 2.10 wB97XD 6-31++g(d.p) -1262.50 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 722.29 2.10 wB97XD cepVVZ -1262.50 -1262.60 -1262.68 -1261.43 -1261.54 -1261.68 716.76 1.45 wB97XD AUG-cepVDZ -1262.52 -1262.63 -1262.43 -1261.49 -1261.55 -1261.68 712.61 716.63 718.63 718.63 1.85 wB97XD AUG-cepVDZ -1262.51	wB97XD		-1248.76	-1248.98	-1249.19	-1248.09	-1248.17	-1248.33	542.88	23.26
wB97XD 6-31g(dp) -1262.31 -1262.46 -1262.65 -1261.33 -1261.33 -1261.51 715.85 1.19 wB97XD 6-31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 722.29 2.10 wB97XD 6-31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 722.29 2.10 wB97XD 6-31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.33 -1261.63 -1261.61 722.29 2.10 wB97XD c-pVDZ -1262.55 -1262.66 -1261.34 -1261.64 -1261.68 7166.81 7	wB97XD	6-31g		-1262.46	-1262.65	-1261.31	-1261.37	-1261.51	715.50	1.14
wB97XD 6-31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g(d,p) -1262.52 -126.60 -126.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD 6-31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.53 -1261.61 722.29 2.10 wB97XD copVDZ -1262.52 -1262.64 -1262.66 -1261.30 -1261.53 -1261.68 719.84 1.76 wB97XD copVDZ -1262.51 -1262.64 -1262.83 -1261.49 -1261.55 -1261.68 717.67 1.45 wB97XD AUG-copVDZ -1262.50 -1262.65 -1262.83 -1261.49 -1261.55 -1261.68 718.03 1.59 wB97XD AUG-copVDZ -1262.50 -1262.65 -1262.83 -1261.49 -1261.55 -1261.68 718.15 1.66 wB97XD AUG-copVDZ -1262.50 -1262.51 -1262.65	wB97XD	6-31g(d,p)			-1262.65	-1261.31	-1261.33			1.19
wB9TXD 6.31+g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 722.99 2.10 wB9TXD 6.31++g(d,p) -1262.52 -1262.60 -1262.66 -1261.30 -1261.51 722.99 2.10 wB9TXD cc-pVDZ -1262.50 -1262.64 -1261.88 -1261.54 -1261.68 717.67 1.45 wB9TXD cc-pVDZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.54 -1261.68 717.67 1.45 wB9TXD AUG-cc-pVDZ -1262.52 -1262.66 -1262.83 -1261.49 -1261.54 -1261.68 718.63 1.59 wB9TXD AUG-cc-pVDZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.54 -1261.68 718.21 1.53 wB9TXD AUG-cc-pVDZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.55 -1261.68 718.61 718.15 1.66 wB9TXD AUG-cc-pVDZ -1262.50 -1262.54 -1262.64 -1261.52<	wB97XD		-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	721.97	2.06
wB97XD 6-31++gd,pl -1262.52 -1262.60 -1262.66 -1261.30 -1261.33 -1261.51 721.97 2.06 wB97XD cc-pVDZ -1262.50 -1262.66 -1262.82 -1261.48 -1261.54 -1261.68 719.84 1.76 wB97XD cc-pVDZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.54 -1261.68 717.67 1.45 wB97XD Cc-pVQZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.55 -1261.69 718.63 1.59 wB97XD AUG-cc-pVDZ -1262.50 -1262.64 -1262.83 -1261.48 -1261.65 -1261.68 718.23 1.53 wB97XD AUG-cc-pVZ -1262.50 -1262.65 -1262.83 -1261.48 -1261.55 -1261.68 718.21 1.53 wB97XD AUG-cc-pVQZ -1262.50 -1262.64 -1261.48 -1261.55 -1261.68 718.61 1.53 wB97XD AUG-cc-pVQZ -1262.50 -1262.54 -1262.64 -1261.26	wB97XD		-1262.52			-1261.30	-1261.33		722.29	2.10
wB97XD 6:31++g(d,p) -1262.50 -1262.64 -1262.82 -1261.33 -1261.33 -1261.68 719.44 1.76 wB97XD ccpVTZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.64 -1261.68 717.67 1.45 wB97XD CcpVCZ -1262.50 -1262.65 -1262.83 -1261.49 -1261.55 -1261.68 717.67 1.45 wB97XD AUG-ccpVDZ -1262.50 -1262.64 -1262.83 -1261.49 -1261.55 -1261.68 718.63 1.59 wB97XD AUG-ccpVDZ -1262.51 -1262.66 -1262.83 -1261.49 -1261.55 -1261.68 718.21 1.53 wB97XD AUG-ccpVZ -1262.51 -1262.66 -1262.83 -1261.49 -1261.55 -1261.68 718.21 1.53 wB97XD AUG-ccpVZ -1262.51 -1262.64 -1262.64 -1261.25 -1261.38 -1261.48 725.70 2.58 wB97XD TZV -1262.60 -1262.44 -1262.64	wB97XD	6-31++g				-1261.30	-1261.33	-1261.51	721.97	2.06
wB97XD cc_PVDZ -1262.61 -1262.65 -1262.82 -1261.48 -1261.54 -1261.68 719.84 1.76 wB97XD cc_PVQZ -1262.51 -1262.65 -1262.83 -1261.49 -1261.55 -1261.68 717.67 1.45 wB97XD AUG-cc-pVZ -1262.50 -1262.65 -1262.83 -1261.48 -1261.55 -1261.68 718.63 1.59 wB97XD AUG-cc-pVZZ -1262.50 -1262.65 -1262.83 -1261.48 -1261.55 -1261.68 718.12 1.53 wB97XD AUG-cc-pVQZ -1262.50 -1262.65 -1262.83 -1261.48 -1261.55 -1261.68 718.12 1.56 wB97XD SVP -1262.50 -1262.64 -1262.65 -1262.64 -1261.38 -1261.48 725.70 2.58 wB97XD SVP -1262.50 -1262.64 -1262.63 -1261.43 -1261.35 -1261.69 719.15 1.66 wB97XD TZVP -1262.66 -1262.70 -1262.83 -1261.	wB97XD	6-31++g(d,p)	-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	722.29	2.10
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wB97XD AUG-cc-pVDZ -1262.50 -1262.64 -1262.83 -1261.68 -1261.65 -1261.65 -1261.65 -1261.65 -1261.65 -1261.65 -1261.65 -1261.65 -1261.65 -1261.68 718.21 1.53 wB97XD AUG-cc-pVQZ -1262.50 -1262.50 -1262.64 -1261.49 -1261.55 -1261.69 719.15 1.66 wB97XD SVP -1262.50 -1262.64 -1261.26 -1261.84 72.51 2.22 wB97XD TZV -1262.66 -1262.70 -1262.80 -1261.43 -1261.66 716.31 1.26 wB97XD QZVP -1262.66 -1262.70 -1262.80 -1261.44 -1261.66 716.31 1.26 wB97XD QZVP -1262.51 -1262.65 -1262.80 -1261.44 -1261.66 -1261.66 716.40 1.27 wB97XD def2SVP -1262.50 -1262.54 -1262.64 -1261.30 -1261.48 723.15 2.22 wB97XD def2SVP -1262.50	wB97XD	cc-pVTZ	-1262.51	-1262.65	-1262.83	-1261.49	-1261.54	-1261.68	717.67	1.45
WB97XD	wB97XD			-1262.65		-1261.49	-1261.55	-1261.69	718.63	1.59
WB97XD	wB97XD			-1262.64		-1261.48		-1261.68		1.81
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LC-wHPBE def2SVPP -1262.26 -1262.31 -1262.41 -1261.01 -1261.06 -1261.24 733.56 3.70										

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
LC-wHPBE	def2TZVP	-1262.42	-1262.47	-1262.58	-1261.19	-1261.23	-1261.42	726.81	2.74
LC-wHPBE	def2TZVPP	-1262.42	-1262.47	-1262.58	-1261.19	-1261.24	-1261.42	727.82	2.88
LC-wHPBE	def2QZV	-1262.45	-1262.50	-1262.60	-1261.21	-1261.35	-1261.45	727.53	2.84
LC-wHPBE	def2QZVP	-1262.45	-1262.50	-1262.61	-1261.21	-1261.35	-1261.45	728.67	3.00
LC-wHPBE	def2QZVPP	-1262.45	-1262.50	-1262.61	-1261.21	-1261.26	-1261.45	728.26	2.95
CAM-B3LYP		-1248.88	-1248.98	-1249.19	-1248.05	-1248.12	-1248.29	562.65	20.46
CAM-B3LYP	6-31g	-1262.34	-1262.49	-1262.68	-1261.33	-1261.39	-1261.54	719.62	1.72
CAM-B3LYP	6-31g(d,p)	-1262.34	-1262.49	-1262.68	-1261.34	-1261.39	-1261.54	719.93	1.77
CAM-B3LYP	6-31+g	-1262.55	-1262.64	-1262.70	-1261.33	-1261.35	-1261.54	727.37	2.82
CAM-B3LYP	6-31+g(d,p)	-1262.55	-1262.64	-1262.70	-1261.33	-1261.36	-1261.54	727.67	2.86
CAM-B3LYP	6-31++g	-1262.55	-1262.64	-1262.70	-1261.33	-1261.35	-1261.54	727.37	2.82
CAM-B3LYP	6-31++g(d,p)	-1262.55	-1262.64	-1262.70	-1261.33	-1261.36	-1261.54	727.67	2.86
CAM-B3LYP	cc-pVDZ	-1262.53	-1262.68	-1262.86	-1261.50	-1261.56	-1261.70	727.86	2.89
CAM-B3LYP	cc-pVTZ	-1262.72	-1262.76	-1262.87	-1261.48	-1261.53	-1261.71	726.53	2.70
CAM-B3LYP	cc-pVQZ	-1262.55	-1262.69	-1262.87	-1261.52	-1261.53	-1261.71	726.88	2.75
CAM-B3LYP	AUG-cc-pVDZ	-1262.53	-1262.68	-1262.86	-1261.50	-1261.52	-1261.70	728.01	2.91
CAM-B3LYP	AUG-cc-pVTZ	-1262.55	-1262.69	-1262.87	-1261.51	-1261.57	-1261.71	726.78	2.74
CAM-B3LYP	AUG-cc-pVQZ	-1262.55	-1262.69	-1262.87	-1261.52	-1261.57	-1261.71	727.11	2.78
CAM-B3LYP	SV	-1262.53	-1262.57	-1262.67	-1261.27	-1261.40	-1261.50	734.59	3.84
CAM-B3LYP	SVP	-1262.53	-1262.57	-1262.67	-1261.28	-1261.40	-1261.50	733.04	3.62
CAM-B3LYP	TZV	-1262.69	-1262.73	-1262.84	-1261.45	-1261.49	-1261.68	724.90	2.47
CAM-B3LYP	TZVP	-1262.69	-1262.74	-1262.84	-1261.45	-1261.58	-1261.68	725.16	2.51
CAM-B3LYP	QZVP	-1262.55	-1262.69	-1262.87	-1261.51	-1261.57	-1261.71	726.91	2.75
CAM-B3LYP	def2SV	-1262.53	-1262.57	-1262.67	-1261.28	-1261.40	-1261.50	733.04	3.62
CAM-B3LYP	def2SVP	-1262.53	-1262.57	-1262.67	-1261.28	-1261.32	-1261.50	733.41	3.67
CAM-B3LYP	def2SVPP	-1262.53	-1262.57	-1262.67	-1261.28	-1261.40	-1261.50	732.77	3.58
CAM-B3LYP	def2TZV	-1262.69	-1262.73	-1262.84	-1261.45	-1261.50	-1261.68	724.77	2.45
CAM-B3LYP	def2TZVP	-1262.69	-1262.74	-1262.84	-1261.46	-1261.58	-1261.68	725.57	2.57
CAM-B3LYP	def2TZVPP	-1262.69	-1262.74	-1262.84	-1261.46	-1261.50	-1261.68	725.84	2.60
CAM-B3LYP	def2QZV	-1262.53	-1262.68	-1262.87	-1261.51	-1261.57	-1261.71	725.72	2.59
CAM-B3LYP	def2QZVP	-1262.55	-1262.69	-1262.87	-1261.51	-1261.53	-1261.71	726.91	2.75
CAM-B3LYP	def2QZVPP	-1262.55	-1262.69	-1262.87	-1261.51	-1261.57	-1261.71	727.00	2.77
wB97XD	4012 422 711	-1248.76	-1248.98	-1249.19	-1248.09	-1248.17	-1248.33	542.88	23.26
wB97XD	6-31g	-1262.31	-1262.46	-1262.65	-1261.31	-1261.37	-1261.51	715.50	1.14
wB97XD	6-31g(d,p)	-1262.31	-1262.46	-1262.65	-1261.31	-1261.33	-1261.51	715.85	1.19
wB97XD	6-31+g	-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	721.97	2.06
wB97XD	6-31+g(d,p)	-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	722.29	2.10
wB97XD	6-31++g	-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	721.97	2.06
wB97XD	6-31++g(d,p)	-1262.52	-1262.60	-1262.66	-1261.30	-1261.33	-1261.51	722.29	2.10
wB97XD	cc-pVDZ	-1262.50	-1262.64	-1262.82	-1261.48	-1261.54	-1261.68	719.84	1.76
wB97XD	cc-pVTZ	-1262.51	-1262.65	-1262.83	-1261.49	-1261.54	-1261.68	717.67	1.45
wB97XD	cc-pVQZ	-1262.52	-1262.65	-1262.83	-1261.49	-1261.55	-1261.69	718.63	1.59
wB97XD	AUG-cc-pVDZ	-1262.50	-1262.64	-1262.83	-1261.48	-1261.54	-1261.68	720.23	1.81
wB97XD	AUG-cc-pVTZ	-1262.51	-1262.65	-1262.83	-1261.49	-1261.55	-1261.68	718.21	1.53
wB97XD	AUG-cc-pVQZ	-1262.52	-1262.65	-1262.83	-1261.49	-1261.55	-1261.69	719.15	1.66
wB97XD	SV SV	-1262.50	-1262.54	-1262.64	-1261.25	-1261.38	-1261.48	725.70	2.58
wB97XD	SVP	-1262.50	-1262.54	-1262.64	-1261.26	-1261.38	-1261.48	723.15	2.22
wB97XD	TZV	-1262.66	-1262.70	-1262.80	-1261.43	-1261.55	-1261.66	716.31	1.26
wB97XD	TZVP	-1262.66	-1262.70	-1262.80	-1261.44	-1261.56	-1261.66	716.40	1.27
wB97XD	QZVP	-1262.51	-1262.65	-1262.83	-1261.49	-1261.51	-1261.68	718.09	1.51
wB97XD	def2SV	-1262.50	-1262.54	-1262.64	-1261.26	-1261.30	-1261.48	722.61	2.15
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Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
wB97XD	def2SVP	-1262.50	-1262.54	-1262.64	-1261.26	-1261.30	-1261.48	723.78	2.31
wB97XD	def2SVPP	-1262.50	-1262.54	-1262.64	-1261.26	-1261.38	-1261.48	723.15	2.22
wB97XD	def2TZV	-1262.66	-1262.70	-1262.80	-1261.43	-1261.48	-1261.66	716.31	1.26
wB97XD	def2TZVP	-1262.66	-1262.70	-1262.80	-1261.44	-1261.56	-1261.66	716.90	1.34
wB97XD	def2TZVPP	-1262.66	-1262.70	-1262.80	-1261.44	-1261.48	-1261.66	717.24	1.39
wB97XD	def2QZV	-1262.49	-1262.64	-1262.83	-1261.49	-1261.50	-1261.68	716.89	1.34
wB97XD	def2QZVP	-1262.51	-1262.65	-1262.83	-1261.49	-1261.51	-1261.68	718.09	1.51
wB97XD	def2QZVPP	-1262.51	-1262.65	-1262.83	-1261.49	-1261.55	-1261.68	718.16	1.52
MN15		-1247.04	-1247.18	-1247.38	-1246.22	-1246.30	-1246.52	538.73	23.85
MN15	6-31g	-1262.56	-1262.64	-1262.73	-1261.33	-1261.45	-1261.59	719.58	1.72
MN15	6-31g(d,p)	-1262.56	-1262.64	-1262.73	-1261.33	-1261.45	-1261.59	719.79	1.75
MN15	6-31+g	-1262.58	-1262.66	-1262.75	-1261.34	-1261.45	-1261.59	726.21	2.66
MN15	6-31+g(d,p)	-1262.58	-1262.66	-1262.75	-1261.34	-1261.46	-1261.59	726.42	2.69
MN15	6-31++g	-1262.58	-1262.66	-1262.75	-1261.34	-1261.45	-1261.59	726.21	2.66
MN15	6-31++g(d,p)	-1262.58	-1262.66	-1262.75	-1261.34	-1261.46	-1261.59	726.42	2.69
MN15	cc-pVDZ	-1262.75	-1262.78	-1262.92	-1261.51	-1261.63	-1261.76	723.42	2.26
MN15	cc-pVTZ	-1262.77	-1262.80	-1262.93	-1261.53	-1261.64	-1261.78	724.47	2.41
MN15	cc-pVQZ	-1262.79	-1262.86	-1262.95	-1261.55	-1261.66	-1261.80	725.77	2.59
MN15	AUG-cc-pVDZ	-1262.75	-1262.78	-1262.92	-1261.51	-1261.58	-1261.76	723.50	2.27
MN15	AUG-cc-pVTZ	-1262.77	-1262.80	-1262.93	-1261.53	-1261.64	-1261.78	724.48	2.41
MN15	AUG-cc-pVQZ	-1262.79	-1262.82	-1262.95	-1261.55	-1261.66	-1261.80	725.76	2.59
MN15	SV	-1262.54	-1262.62	-1262.71	-1261.28	-1261.40	-1261.54	732.21	3.50
MN15	SVP	-1262.54	-1262.62	-1262.71	-1261.29	-1261.41	-1261.55	730.30	3.23
MN15	TZV	-1262.73	-1262.80	-1262.89	-1261.49	-1261.61	-1261.74	721.36	1.97
MN15	TZVP	-1262.73	-1262.81	-1262.89	-1261.49	-1261.61	-1261.74	721.85	2.04
MN15	QZVP	-1262.81	-1262.89	-1262.97	-1261.57	-1261.69	-1261.82	724.81	2.46
MN15	def2SV	-1262.54	-1262.62	-1262.71	-1261.29	-1261.41	-1261.55	730.30	3.23
MN15	def2SVP	-1262.54	-1262.62	-1262.71	-1261.29	-1261.41	-1261.55	730.76	3.30
MN15	def2SVPP	-1262.54	-1262.62	-1262.71	-1261.29	-1261.41	-1261.55	730.30	3.23
MN15	def2TZV	-1262.73	-1262.80	-1262.89	-1261.49	-1261.61	-1261.74	721.36	1.97
MN15	def2TZVP	-1262.73	-1262.81	-1262.90	-1261.49	-1261.61	-1261.74	721.98	2.06
MN15	def2TZVPP	-1262.73	-1262.81	-1262.90	-1261.50	-1261.61	-1261.75	722.87	2.18
MN15	def2QZV	-1262.81	-1262.88	-1262.97	-1261.57	-1261.68	-1261.82	723.68	2.30
MN15	def2QZVP	-1262.81	-1262.89	-1262.97	-1261.57	-1261.69	-1261.82	724.81	2.46
MN15	def2QZVPP	-1262.81	-1262.89	-1262.98	-1261.57	-1261.69	-1261.82	724.93	2.47
M11		-1248.27	-1248.49	-1248.69	-1247.59	-1247.61	-1247.82	546.22	22.79
M11	6-31g	-1262.36	-1262.42	-1262.52	-1261.14	-1261.25	-1261.38	718.46	1.56
M11	6-31g(d,p)	-1262.36	-1262.42	-1262.52	-1261.14	-1261.25	-1261.38	718.73	1.60
M11	6-31+g	-1262.38	-1262.44	-1262.54	-1261.14	-1261.25	-1261.38	725.94	2.62
M11	6-31+g(d,p)	-1262.38	-1262.44	-1262.54	-1261.14	-1261.25	-1261.38	726.20	2.65
M11	6-31++g	-1262.38	-1262.44	-1262.54	-1261.14	-1261.25	-1261.38	725.94	2.62
M11	6-31++g(d,p)	-1262.38	-1262.44	-1262.54	-1261.14	-1261.25	-1261.38	726.20	2.65
M11	cc-pVDZ	-1262.55	-1262.57	-1262.71	-1261.32	-1261.43	-1261.55	725.32	2.53
M11	cc-pVTZ	-1262.55	-1262.57	-1262.71	-1261.32	-1261.39	-1261.56	723.21	2.23
M11	cc-pVIZ	-1262.56	-1262.62	-1262.71	-1261.33	-1261.44	-1261.57	723.66	2.30
M11	AUG-cc-pVDZ	-1262.55	-1262.61	-1262.72	-1261.32	-1261.43	-1261.55	725.23	2.52
M11	AUG-cc-pVTZ	-1262.55	-1262.61	-1262.71	-1261.32	-1261.43	-1261.56	723.22	2.32
M11	AUG-cc-pVQZ	-1262.56	-1262.62	-1262.71	-1261.33	-1261.44	-1261.57	723.66	2.30
M11	SV SV	-1262.35	-1262.42	-1262.72	-1261.11	-1261.22	-1261.35	728.98	3.05
M11	SVP	-1262.35	-1262.42	-1262.51	-1261.11	-1261.22	-1261.36	727.24	2.80
M11	TZV	-1262.55	-1262.42	-1262.51	-1261.12	-1261.23	-1261.36	720.81	1.89
17111	IZV	-1202.32	-1202.08	-1202.08	-1201.30	-1201.40	-1201.03	120.01	1.09

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
M11	TZVP	-1262.52	-1262.59	-1262.68	-1261.30	-1261.40	-1261.54	720.94	1.91
M11	QZVP	-1262.56	-1262.62	-1262.72	-1261.33	-1261.39	-1261.56	723.62	2.29
M11	def2SV	-1262.35	-1262.42	-1262.51	-1261.12	-1261.23	-1261.36	727.24	2.80
M11	def2SVP	-1262.35	-1262.42	-1262.52	-1261.12	-1261.23	-1261.36	727.77	2.88
M11	def2SVPP	-1262.35	-1262.42	-1262.51	-1261.12	-1261.23	-1261.36	727.24	2.80
M11	def2TZV	-1262.52	-1262.58	-1262.68	-1261.30	-1261.40	-1261.53	720.81	1.89
M11	def2TZVP	-1262.52	-1262.59	-1262.69	-1261.30	-1261.41	-1261.54	721.33	1.97
M11	def2TZVPP	-1262.52	-1262.59	-1262.69	-1261.30	-1261.36	-1261.54	721.84	2.04
M11	def2QZV	-1262.56	-1262.62	-1262.72	-1261.33	-1261.43	-1261.56	722.49	2.13
M11	def2QZVP	-1262.56	-1262.62	-1262.72	-1261.33	-1261.44	-1261.56	723.62	2.29
M11	def2QZVPP	-1262.56	-1262.62	-1262.72	-1261.33	-1261.44	-1261.56	723.69	2.30
SOGGA11X	-	-1248.82	-1249.07	-1249.29	-1248.14	-1248.17	-1248.40	557.45	21.20
SOGGA11X	6-31g	-1262.29	-1262.43	-1262.63	-1261.28	-1261.31	-1261.51	703.97	0.49
SOGGA11X	6-31g(d,p)	-1262.29	-1262.44	-1262.63	-1261.28	-1261.35	-1261.51	704.29	0.44
SOGGA11X	6-31+g	-1262.31	-1262.45	-1262.64	-1261.29	-1261.36	-1261.51	709.44	0.29
SOGGA11X	6-31+g(d,p)	-1262.31	-1262.45	-1262.64	-1261.29	-1261.36	-1261.51	709.75	0.33
SOGGA11X	6-31++g	-1262.31	-1262.45	-1262.64	-1261.29	-1261.36	-1261.51	709.44	0.29
SOGGA11X	6-31++g(d,p)	-1262.31	-1262.45	-1262.64	-1261.29	-1261.31	-1261.51	709.75	0.33
SOGGA11X	cc-pVDZ	-1262.47	-1262.62	-1262.81	-1261.45	-1261.47	-1261.66	716.72	1.32
SOGGA11X	cc-pVTZ	-1262.48	-1262.62	-1262.81	-1261.46	-1261.52	-1261.67	714.26	0.97
SOGGA11X	cc-pVQZ	-1262.49	-1262.63	-1262.81	-1261.46	-1261.52	-1261.67	714.81	1.05
SOGGA11X	AUG-cc-pVDZ	-1262.47	-1262.62	-1262.81	-1261.45	-1261.52	-1261.66	716.59	1.30
SOGGA11X	AUG-cc-pVTZ	-1262.48	-1262.62	-1262.81	-1261.46	-1261.52	-1261.67	714.27	0.97
SOGGA11X	AUG-cc-pVQZ	-1262.49	-1262.63	-1262.81	-1261.46	-1261.52	-1261.67	714.82	1.05
SOGGA11X	SV	-1262.47	-1262.42	-1262.62	-1261.22	-1261.27	-1261.46	723.85	2.32
SOGGA11X	SVP	-1262.47	-1262.51	-1262.62	-1261.24	-1261.27	-1261.47	721.91	2.05
SOGGA11X	TZV	-1262.63	-1262.67	-1262.78	-1261.41	-1261.53	-1261.64	713.05	0.80
SOGGA11X	TZVP	-1262.44	-1262.59	-1262.78	-1261.43	-1261.49	-1261.64	713.02	0.79
SOGGA11X	QZVP	-1262.49	-1262.62	-1262.81	-1261.46	-1261.52	-1261.67	714.65	1.02
SOGGA11X	def2SV	-1262.47	-1262.51	-1262.62	-1261.22	-1261.27	-1261.47	721.91	2.05
SOGGA11X	def2SVP	-1262.47	-1262.51	-1262.62	-1261.25	-1261.27	-1261.47	722.63	2.15
SOGGA11X	def2SVPP	-1262.47	-1262.51	-1262.62	-1261.22	-1261.27	-1261.47	721.91	2.05
SOGGA11X	def2TZV	-1262.63	-1262.67	-1262.78	-1261.41	-1261.53	-1261.64	713.05	0.80
SOGGA11X	def2TZVP	-1262.63	-1262.67	-1262.78	-1261.41	-1261.53	-1261.64	713.68	0.89
SOGGA11X	def2TZVPP	-1262.46	-1262.60	-1262.78	-1261.43	-1261.50	-1261.64	714.01	0.93
SOGGA11X	def2QZV	-1262.47	-1262.62	-1262.81	-1261.45	-1261.52	-1261.67	713.34	0.84
SOGGA11X	def2QZVP	-1262.49	-1262.62	-1262.81	-1261.46	-1261.52	-1261.67	714.65	1.02
SOGGA11X	def2QZVPP	-1262.49	-1262.62	-1262.81	-1261.46	-1261.52	-1261.67	714.67	1.03
N12SX		-1247.87	-1248.12	-1248.19	-1247.17	-1247.25	-1247.31	549.96	22.26
N12SX	6-31g	-1262.01	-1261.93	-1262.09	-1260.82	-1260.84	-1260.92	731.38	3.39
N12SX	6-31g(d,p)	-1262.01	-1261.94	-1262.09	-1260.82	-1260.84	-1260.92	731.71	3.43
N12SX	6-31+g	-1262.03	-1261.95	-1262.10	-1260.82	-1260.80	-1260.92	740.50	4.68
N12SX	6-31+g(d,p)	-1262.03	-1261.96	-1262.11	-1260.83	-1260.85	-1260.92	740.79	4.72
N12SX	6-31++g	-1262.03	-1261.95	-1262.10	-1260.82	-1260.84	-1260.92	740.50	4.68
N12SX	6-31++g(d,p)	-1262.03	-1261.96	-1262.11	-1260.83	-1260.80	-1260.92	740.79	4.72
N12SX	cc-pVDZ	-1262.19	-1262.13	-1262.27	-1260.99	-1260.97	-1261.09	742.27	4.93
N12SX	cc-pVTZ	-1262.20	-1262.14	-1262.28	-1261.00	-1261.02	-1261.10	741.33	4.79
N12SX	cc-pVQZ	-1262.21	-1262.15	-1262.29	-1261.01	-1260.99	-1261.11	742.32	4.93
N12SX	AUG-cc-pVDZ	-1262.19	-1262.13	-1262.27	-1261.00	-1261.01	-1261.09	742.77	5.00
N12SX	AUG-cc-pVTZ	-1262.20	-1262.14	-1262.28	-1261.00	-1261.02	-1261.10	741.88	4.87
N12SX	AUG-cc-pVQZ	-1262.21	-1262.15	-1262.29	-1261.01	-1261.03	-1261.11	742.80	5.00

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
N12SX	SV	-1262.00	-1262.02	-1262.08	-1260.76	-1260.76	-1260.89	745.65	5.40
N12SX	SVP	-1262.00	-1262.02	-1262.08	-1260.77	-1260.85	-1260.90	743.81	5.14
N12SX	TZV	-1262.17	-1262.19	-1262.25	-1260.97	-1261.03	-1261.07	740.11	4.62
N12SX	TZVP	-1262.17	-1262.19	-1262.25	-1260.97	-1260.95	-1261.07	740.23	4.64
N12SX	QZVP	-1262.21	-1262.15	-1262.29	-1261.01	-1261.03	-1261.11	741.02	4.75
N12SX	def2SV	-1262.00	-1262.02	-1262.08	-1260.77	-1260.85	-1260.90	743.22	5.06
N12SX	def2SVP	-1262.00	-1262.03	-1262.08	-1260.80	-1260.86	-1260.90	743.93	5.16
N12SX	def2SVPP	-1262.00	-1262.02	-1262.08	-1260.77	-1260.85	-1260.90	743.22	5.06
N12SX	def2TZV	-1262.17	-1262.19	-1262.25	-1260.97	-1261.03	-1261.07	739.56	4.54
N12SX	def2TZVP	-1262.17	-1262.20	-1262.25	-1260.97	-1261.03	-1261.07	740.82	4.72
N12SX	def2TZVPP	-1262.17	-1262.20	-1262.25	-1260.98	-1261.04	-1261.07	741.30	4.79
N12SX	def2QZV	-1262.21	-1262.14	-1262.29	-1261.01	-1261.03	-1261.11	739.65	4.56
N12SX	def2QZVP	-1262.21	-1262.15	-1262.29	-1261.01	-1261.03	-1261.11	741.02	4.75
N12SX	def2QZVPP	-1262.21	-1262.15	-1262.29	-1261.01	-1261.03	-1261.11	741.10	4.76
MN12SX	<u> </u>	-1240.08	-1247.11	-1247.24	-1246.18	-1246.25	-1246.38	536.42	24.17
MN12SX	6-31g	-1262.40	-1262.43	-1262.48	-1261.17	-1261.24	-1261.34	714.14	0.95
MN12SX	6-31g(d,p)	-1262.40	-1262.43	-1262.48	-1261.17	-1261.24	-1261.34	714.67	1.03
MN12SX	6-31+g	-1262.42	-1262.45	-1262.50	-1261.17	-1261.25	-1261.35	724.93	2.48
MN12SX	6-31+g(d,p)	-1262.42	-1262.45	-1262.50	-1261.18	-1261.25	-1261.35	725.44	2.55
MN12SX	6-31++g	-1262.42	-1262.45	-1262.50	-1261.17	-1261.25	-1261.35	724.93	2.48
MN12SX	6-31++g(d,p)	-1262.42	-1262.45	-1262.50	-1261.18	-1261.25	-1261.35	725.44	2.55
MN12SX	cc-pVDZ	-1262.58	-1262.56	-1262.67	-1261.34	-1261.41	-1261.51	725.46	2.55
MN12SX	cc-pVTZ	-1262.59	-1262.62	-1262.68	-1261.35	-1261.42	-1261.52	725.62	2.57
MN12SX	cc-pVQZ	-1262.60	-1262.58	-1262.69	-1261.36	-1261.43	-1261.53	727.20	2.80
MN12SX	AUG-cc-pVDZ	-1262.58	-1262.56	-1262.67	-1261.34	-1261.41	-1261.51	725.45	2.55
MN12SX	AUG-cc-pVTZ	-1262.59	-1262.62	-1262.68	-1261.35	-1261.42	-1261.52	725.64	2.58
MN12SX	AUG-cc-pVQZ	-1262.60	-1262.63	-1262.69	-1261.36	-1261.38	-1261.53	727.23	2.80
MN12SX MN12SX	SV	-1262.36	-1262.39	-1262.44	-1261.11	-1261.18	-1261.29	726.98	2.76
MN12SX	SVP	-1262.36	-1262.39	-1262.45	-1261.12	-1261.19	-1261.29	725.61	2.57
MN12SX	TZV	-1262.56	-1262.59	-1262.64	-1261.32	-1261.39	-1261.49	723.91	2.33
MN12SX	TZVP	-1262.56	-1262.59	-1262.64	-1261.32	-1261.39	-1261.49	723.86	2.32
MN12SX	QZVP	-1262.60	-1262.63	-1262.69	-1261.36	-1261.43	-1261.53	725.94	2.62
MN12SX	def2SV	-1262.36	-1262.39	-1262.45	-1261.12	-1261.19	-1261.29	725.61	2.57
MN12SX	def2SVP	-1262.36	-1262.39	-1262.45	-1261.12	-1261.19	-1261.29	726.74	2.73
MN12SX	def2SVPP	-1262.36	-1262.39	-1262.45	-1261.12	-1261.19	-1261.29	725.61	2.57
MN12SX	def2TZV	-1262.56	-1262.59	-1262.64	-1261.32	-1261.39	-1261.49	723.91	2.33
MN12SX MN12SX	def2TZVP	-1262.56	-1262.59	-1262.64	-1261.32	-1261.39	-1261.49	725.01	2.49
MN12SX MN12SX	def2TZVPP	-1262.56	-1262.59	-1262.65	-1261.33	-1261.34	-1261.49	725.57	2.57
MN12SX MN12SX	def2QZV	-1262.60	-1262.63	-1262.68	-1261.36	-1261.43	-1261.53	724.06	2.35
MN12SX	def2QZVP	-1262.60	-1262.63	-1262.69	-1261.36	-1261.43	-1261.53	725.94	2.62
MN12SX MN12SX	def2QZVPP	-1262.60	-1262.63	-1262.69	-1261.36	-1261.43	-1261.53	725.96	2.62
PW6B95	301242111	-1246.63	-1249.75	-1249.87	-1248.74	-1248.81	-1248.98	557.95	21.13
PW6B95	6-31g	-1263.18	-1263.24	-1263.33	-1261.95	-1262.04	-1262.18	719.05	1.64
PW6B95	6-31g(d,p)	-1263.18	-1263.24	-1263.33	-1261.95	-1262.04	-1262.18	719.37	1.69
PW6B95	6-31+g	-1263.20	-1263.27	-1254.83	-1262.04	-1260.68	-1262.19	676.66	4.35
PW6B95	6-31+g(d,p)	-1233.19	-1263.25	-1254.30	-1262.04	-1262.09	-1262.19	667.55	5.64
PW6B95	6-31++g	-1263.20	-1263.25	-1254.83	-1262.04	-1248.55	-1262.19	667.27	5.68
PW6B95	6-31++g 6-31++g(d,p)	-1233.19	-1263.25	-1254.30	-1262.04	-1249.27	-1262.19	667.55	5.64
PW6B95	cc-pVDZ	-1263.36	-1263.44	-1263.51	-1262.11	-1262.25	-1262.35	726.20	2.66
PW6B95	cc-pVTZ	-1263.36	-1263.38	-1263.51	-1262.11	-1262.25	-1262.36	724.18	2.37
PW6B95	cc-pV1Z	-1263.37	-1263.42	-1263.51	-1262.12	-1262.22	-1262.36	724.16	2.43
1 110090	CC-P / QZ	-1200.01	-1200.42	1200.01	-1202.12	-1202.22	-1202.30	124.01	2.40

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

PW6B95 AUG-cc-pVDZ -1263.36 -1252.98 -1255.64 -1259.76 -1256.85 -1262.35 563.431 PW6B95 AUG-cc-pVTZ -1263.36 -1263.42 -1263.51 -1262.12 -1262.22 -1262.36 724.60 PW6B95 AUG-cc-pVQZ -1263.37 -1263.42 -1263.51 -1262.12 -1262.22 -1262.36 724.60 PW6B95 SV -1263.17 -1263.22 -1263.32 -1261.95 -1262.04 -1262.15 733.44 PW6B95 SVP -1263.17 -1263.22 -1263.32 -1261.95 -1262.04 -1262.15 733.14 PW6B95 SVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1260.48 -1260.09 -1262.19 -1262.33 722.72 PW6B95 def2SV -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVP -1263.17 -1263.23 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVPP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.18 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.63 PW6B95 def2QZV -1263.36 -1263.45 -1263.51 -1262.12 -1262.21 -1262.36 685.22 PW6B95 def2QZV -1263.36 -1263.45 -1263.51 -1262.12 -1262.21 -1262.36 685.22 PW6B95 def2QZV -1263.36 -1263.45 -1263.51 -1262.12 -1262.21 -1262.36 685.22 PW6B95 def2QZVP -1263.36 -1263.45 -1263.51 -1262.12 -1261.32 -1261.46 706.74 M08HX 6-31g -1262.43 -1262.49 -1262.59 -1261.21 -1261.32 -1261.46 707.00 M08HX 6-31+g(d,p) -1262.45 -1262.51 -1262.60 -1261.22 -1261.33 -1261.47 714.08 M08HX Cc-pVDZ -1262.63	10.34 2.37 2.43 3.68 3.35 2.14 2.16 10.59 3.35 3.45 3.35 2.14 2.23 2.29 2.27 3.14 2.41 2.131 0.10 0.06
PW6B95	2.43 3.68 3.35 2.14 2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10
PW6B95 SV -1263.17 -1262.56 -1263.32 -1261.95 -1262.04 -1262.15 733.44 PW6B95 SVP -1263.17 -1263.22 -1263.33 -1261.91 -1262.19 -1262.35 731.15 PW6B95 TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1250.04 -1262.12 -1262.26 -1262.36 632.50 PW6B95 def2SV -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVPP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.18 PW6B95 def2TZVP -12	3.68 3.35 2.14 2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31
PW6B95 SVP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1260.04 -1262.12 -1262.26 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1260.04 -1262.12 -1262.26 -1262.35 632.50 PW6B95 def2SV -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVPP -1263.17 -1263.23 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZV -1263.34 -1263.33 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZV -1263.34 -1263.39 -1263.32 -1262.09 -1262.19 -1262.33 722.54 PW6B95 def2QZV -1263.34 -1263.39 -12	3.35 2.14 2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10
PW6B95 TZV -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 TZVP -1263.34 -1263.38 -1260.09 -1262.19 -1262.36 722.72 PW6B95 QZVP -1263.36 -1260.83 -1250.04 -1262.10 -1262.26 -1263.36 -1260.15 731.15 PW6B95 def2SVP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVP -1263.17 -1263.23 -1261.91 -1262.01 -1262.15 731.79 PW6B95 def2SVP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZV -1263.34 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.48 PW6B95 def2QZV -1263.36 -1263.42 <td< td=""><td>2.14 2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10</td></td<>	2.14 2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10
PW6B95 TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1250.04 -1262.12 -1262.26 -1262.36 632.50 PW6B95 def2SV -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.79 PW6B95 def2TZVV -1263.41 -1263.32 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 def2TZVPP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.18 PW6B95 def2QZV -1263.34 -1263.39 -1263.48 -1262.10 -1262.49 -1262.33 723.18 PW6B95 def2QZVP	2.16 10.59 3.35 3.45 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10
PW6B95 TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 722.72 PW6B95 QZVP -1263.36 -1260.83 -1250.04 -1262.12 -1262.26 -1262.36 632.50 PW6B95 def2SV -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.15 PW6B95 def2SVPP -1263.17 -1263.22 -1263.32 -1261.91 -1262.01 -1262.15 731.79 PW6B95 def2TZVV -1263.34 -1263.32 -1263.48 -1262.09 -1262.19 -1262.33 722.54 PW6B95 def2TZVP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.18 PW6B95 def2TZVPP -1263.34 -1263.39 -1263.48 -1262.09 -1262.19 -1262.33 723.18 PW6B95 def2QZV -1263.36 -1263.42 -1263.51 -1262.12 -1262.21 -1262.33 723.49 PW6B95 def2QZVP	10.59 3.35 3.45 3.35 2.14 2.23 2.29 2.27 3.14 2.41 21.31 0.10
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M08HX cc-pVDZ -1262.62 -1262.63 -1262.78 -1261.39 -1261.44 -1261.64 715.13 M08HX cc-pVTZ -1262.62 -1262.64 -1262.78 -1261.40 -1261.50 -1261.64 713.13 M08HX cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.66 M08HX AUG-cc-pVDZ -1262.62 -1262.63 -1262.78 -1261.39 -1261.44 -1261.64 715.05 M08HX AUG-cc-pVTZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP	0.94
M08HX cc-pVTZ -1262.62 -1262.64 -1262.78 -1261.40 -1261.50 -1261.64 713.13 M08HX cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.66 M08HX AUG-cc-pVDZ -1262.62 -1262.63 -1262.78 -1261.39 -1261.44 -1261.64 715.05 M08HX AUG-cc-pVTZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX SV -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX TZV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262	
M08HX cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.66 M08HX AUG-cc-pVDZ -1262.62 -1262.63 -1262.78 -1261.39 -1261.44 -1261.64 715.05 M08HX AUG-cc-pVTZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.	1.09
M08HX AUG-cc-pVDZ -1262.62 -1262.63 -1262.78 -1261.39 -1261.44 -1261.64 715.05 M08HX AUG-cc-pVTZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.81
M08HX AUG-cc-pVTZ -1262.62 -1262.68 -1262.78 -1261.40 -1261.50 -1261.64 713.14 M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.88
M08HX AUG-cc-pVQZ -1262.63 -1262.69 -1262.78 -1261.40 -1261.45 -1261.65 713.67 M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	1.08
M08HX SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.44 719.94 M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.81
M08HX SVP -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01 M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.88
M08HX TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57 M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	1.77
M08HX TZVP -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.68 M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	1.50
M08HX QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.59
	0.60
	0.85
M08HX def2SV -1262.43 -1262.49 -1262.59 -1261.19 -1261.30 -1261.45 718.01	1.50
M08HX def2SVP -1262.43 -1262.50 -1262.59 -1261.19 -1261.30 -1261.45 718.47	1.56
M08HX def2SVPP -1262.43 -1262.49 -1262.59 -1261.19 -1261.25 -1261.45 718.01	1.50
M08HX def2TZV -1262.59 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 711.57	0.59
M08HX def2TZVP -1262.60 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 712.04	0.65
M08HX def2TZVPP -1262.60 -1262.66 -1262.75 -1261.37 -1261.48 -1261.62 712.52	0.72
M08HX def2QZV -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 712.37	0.70
M08HX def2QZVP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.41	0.85
M08HX def2QZVPP -1262.63 -1262.69 -1262.78 -1261.40 -1261.51 -1261.65 713.49	0.86
M06 -1241.71 -1248.92 -1249.11 -1247.94 -1248.03 -1248.25 541.75	23.42
M06 6-31g -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.45 704.08	0.47
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	0.44
M06 6-31+g -1262.43 -1262.49 -1262.58 -1261.17 -1261.28 -1261.45 711.07	0.52
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	
M06 6-31++g -1262.43 -1262.49 -1262.58 -1261.17 -1261.28 -1261.45 711.07	0.55
M06 $6-31++g(d,p)$ -1262.43 -1262.49 -1262.58 -1261.17 -1261.28 -1261.45 711.28	

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
M06	cc-pVDZ	-1262.58	-1262.60	-1262.74	-1261.33	-1261.44	-1261.61	708.65	0.17
M06	cc-pVTZ	-1262.59	-1262.60	-1262.74	-1261.34	-1261.45	-1261.62	706.29	0.16
M06	cc-pVQZ	-1262.59	-1262.60	-1262.75	-1261.34	-1261.45	-1261.62	707.45	0.00
M06	AUG-cc-pVDZ	-1262.58	-1262.60	-1262.74	-1261.33	-1261.44	-1261.61	708.54	0.16
M06	AUG-cc-pVTZ	-1262.59	-1262.60	-1262.74	-1261.34	-1261.45	-1261.62	706.32	0.16
M06	AUG-cc-pVQZ	-1262.59	-1262.65	-1262.75	-1261.34	-1261.45	-1261.62	707.47	0.01
M06	SV	-1262.39	-1262.45	-1262.54	-1261.12	-1261.23	-1261.41	713.10	0.80
M06	SVP	-1262.39	-1262.45	-1262.55	-1261.13	-1261.24	-1261.41	710.20	0.39
M06	TZV	-1262.56	-1262.62	-1262.72	-1261.31	-1261.42	-1261.59	705.37	0.29
M06	TZVP	-1262.56	-1262.62	-1262.72	-1261.31	-1261.42	-1261.59	705.35	0.29
M06	QZVP	-1262.59	-1262.64	-1262.74	-1261.34	-1261.45	-1261.62	706.94	0.07
M06	def2SV	-1262.39	-1262.45	-1262.55	-1261.13	-1261.24	-1261.41	710.20	0.39
M06	def2SVP	-1262.39	-1262.45	-1262.55	-1261.13	-1261.24	-1261.41	710.63	0.45
M06	def2SVPP	-1262.39	-1262.45	-1262.55	-1261.13	-1261.24	-1261.41	710.20	0.39
M06	def2TZV	-1262.56	-1262.62	-1262.72	-1261.31	-1261.42	-1261.59	705.37	0.29
M06	def2TZVP	-1262.56	-1262.62	-1262.72	-1261.31	-1261.42	-1261.59	705.73	0.24
M06	def2TZVPP	-1262.56	-1262.62	-1262.72	-1261.31	-1261.38	-1261.59	705.83	0.24
M06	def2QZV	-1262.59	-1262.64	-1262.74	-1261.34	-1261.45	-1261.62	706.12	0.18
M06	def2QZVP	-1262.59	-1262.64	-1262.74	-1261.34	-1261.45	-1261.62	706.12	0.13
M06	def2QZVPP	-1262.59	-1262.65	-1262.74	-1261.34	-1261.45	-1261.62	706.99	0.07
M062X	deizQZVII	-1202.33	-1248.94	-1202.74	-1247.82	-1248.10	-1248.28	561.60	20.61
M062X M062X	6-31g	-1248.72	-1248.94	-1249.17	-1247.82	-1248.10	-1246.26	711.03	0.51
	6-31g(d,p)	-1262.44	-1262.50	-1262.59	-1261.21	-1261.32	-1261.46	711.03	0.55
M062X M062X	6-31+g	-1262.44	-1262.51	-1262.59	-1261.21	-1261.32	-1261.46	716.99	1.35
	6-31+g 6-31+g(d,p)			-1262.61					
M062X		-1262.45	-1262.51		-1261.22	-1261.32	-1261.46	717.28	1.39
M062X	6-31++g	-1262.45	-1262.51	-1262.61	-1261.22	-1261.32	-1261.46	716.99	1.35
M062X	6-31++g(d,p)	-1262.45	-1262.51	-1262.61	-1261.22	-1261.32	-1261.46	717.28	1.39
M062X	cc-pVDZ	-1262.62	-1262.63	-1262.77	-1261.38	-1261.44	-1261.63	713.98	0.93
M062X	cc-pVTZ	-1262.62	-1262.64	-1262.77	-1261.39	-1261.49	-1261.64	712.11	0.66
M062X	cc-pVQZ	-1262.62	-1262.68	-1262.78	-1261.39	-1261.50	-1261.64	713.08	0.80
M062X	AUG-cc-pVDZ	-1262.62	-1262.63	-1262.77	-1261.38	-1261.49	-1261.63	713.86	0.91
M062X	AUG-cc-pVTZ	-1262.62	-1262.68	-1262.77	-1261.39	-1261.49	-1261.64	712.14	0.67
M062X	AUG-cc-pVQZ	-1262.62	-1262.64	-1262.78	-1261.39	-1261.50	-1261.64	713.09	0.80
M062X	SV	-1262.43	-1262.49	-1262.58	-1261.18	-1261.29	-1261.44	720.17	1.80
M062X	SVP	-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	718.25	1.53
M062X	TZV	-1262.59	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	710.13	0.38
M062X	TZVP	-1262.59	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	710.35	0.41
M062X	QZVP	-1262.62	-1262.68	-1262.78	-1261.39	-1261.50	-1261.64	712.88	0.77
M062X	def2SV	-1262.43	-1262.49	-1262.59	-1261.19	-1261.25	-1261.44	718.25	1.53
M062X	def2SVP	-1262.43	-1262.49	-1262.59	-1261.19	-1261.25	-1261.44	718.77	1.60
M062X	def2SVPP	-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	718.25	1.53
M062X	def2TZV	-1262.59	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	710.13	0.38
M062X	def2TZVP	-1262.59	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	710.70	0.46
M062X	def2TZVPP	-1262.59	-1262.65	-1262.75	-1261.37	-1261.43	-1261.61	711.08	0.52
M062X	def2QZV	-1262.62	-1262.68	-1262.78	-1261.39	-1261.49	-1261.64	711.90	0.63
M062X	def2QZVP	-1262.62	-1262.68	-1262.78	-1261.39	-1261.50	-1261.64	712.88	0.77
M062X	def2QZVPP	-1262.62	-1262.64	-1262.78	-1261.39	-1261.50	-1261.64	712.95	0.78
M05		-1248.95	-1249.25	-1249.42	-1248.23	-1248.32	-1248.53	555.29	21.50
M05	6-31g	-1262.47	-1262.54	-1262.65	-1261.23	-1261.35	-1261.53	702.76	0.66
MOS									
M05	6-31g(d,p)	-1262.48	-1262.54	-1262.65	-1261.23	-1261.35	-1261.53	702.97	0.63

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
M05	6-31+g(d,p)	-1262.49	-1262.56	-1262.67	-1261.24	-1261.36	-1261.53	710.25	0.40
M05	6-31++g	-1262.49	-1262.56	-1262.67	-1261.24	-1261.36	-1261.53	710.05	0.37
M05	6-31++g(d,p)	-1262.49	-1262.56	-1262.67	-1261.24	-1261.36	-1261.53	710.25	0.40
M05	cc-pVDZ	-1262.65	-1262.67	-1262.82	-1261.40	-1261.51	-1261.69	712.37	0.70
M05	cc-pVTZ	-1262.65	-1262.68	-1262.83	-1261.40	-1261.52	-1261.69	710.06	0.37
M05	cc-pVQZ	-1262.65	-1262.72	-1262.83	-1261.41	-1261.52	-1261.70	710.07	0.37
M05	AUG-cc-pVDZ	-1262.65	-1262.67	-1262.82	-1261.40	-1261.47	-1261.69	712.28	0.69
M05	AUG-cc-pVTZ	-1262.65	-1262.68	-1262.83	-1261.40	-1261.52	-1261.69	710.09	0.38
M05	AUG-cc-pVQZ	-1262.65	-1262.72	-1262.83	-1261.41	-1261.52	-1261.70	710.08	0.38
M05	SV	-1262.46	-1262.53	-1262.64	-1261.20	-1261.32	-1261.50	715.88	1.20
M05	SVP	-1262.46	-1262.53	-1262.64	-1261.20	-1261.32	-1261.50	713.57	0.87
M05	TZV	-1262.62	-1262.69	-1262.80	-1261.37	-1261.49	-1261.67	709.40	0.28
M05	TZVP	-1262.62	-1262.69	-1262.80	-1261.37	-1261.49	-1261.67	709.50	0.29
M05	QZVP	-1262.65	-1262.72	-1262.83	-1261.40	-1261.52	-1261.70	709.94	0.36
M05	def2SV	-1262.46	-1262.53	-1262.64	-1261.20	-1261.32	-1261.50	713.57	0.87
M05	def2SVP	-1262.46	-1262.53	-1262.64	-1261.20	-1261.32	-1261.50	714.01	0.93
M05	def2SVPP	-1262.46	-1262.53	-1262.64	-1261.20	-1261.32	-1261.50	713.57	0.87
M05	def2TZV	-1262.62	-1262.69	-1262.80	-1261.37	-1261.49	-1261.67	709.40	0.28
M05	def2TZVP	-1262.62	-1262.69	-1262.80	-1261.38	-1261.49	-1261.67	709.95	0.36
M05	def2TZVPP	-1262.63	-1262.69	-1262.80	-1261.38	-1261.46	-1261.67	710.24	0.40
M05	def2QZV	-1262.65	-1262.72	-1262.83	-1261.40	-1261.52	-1261.70	709.07	0.23
M05	def2QZVP	-1262.65	-1262.72	-1262.83	-1261.40	-1261.52	-1261.70	709.94	0.36
M05	def2QZVPP	-1262.65	-1262.72	-1262.83	-1261.40	-1261.52	-1261.70	709.99	0.36
M052X	401242711	-1248.74	-1248.96	-1249.18	-1247.85	-1248.08	-1248.30	553.07	21.82
M052X	6-31g	-1262.40	-1262.46	-1262.57	-1261.18	-1261.29	-1261.43	712.01	0.65
M052X	6-31g(d,p)	-1262.40	-1262.46	-1262.57	-1261.18	-1261.29	-1261.43	712.31	0.69
M052X	6-31+g	-1262.41	-1262.48	-1262.58	-1261.18	-1261.29	-1261.44	717.75	1.46
M052X	6-31+g(d,p)	-1262.41	-1262.48	-1262.58	-1261.18	-1261.29	-1261.44	718.03	1.50
M052X	6-31++g	-1262.41	-1262.48	-1262.58	-1261.18	-1261.29	-1261.44	717.75	1.46
M052X	6-31++g(d,p)	-1262.41	-1262.48	-1262.58	-1261.18	-1261.29	-1261.44	718.03	1.50
M052X	cc-pVDZ	-1262.58	-1262.60	-1262.74	-1261.35	-1261.42	-1261.60	715.73	1.17
M052X	cc-pVTZ	-1262.58	-1262.64	-1262.75	-1261.35	-1261.46	-1261.61	713.82	0.90
M052X	cc-pVIZ	-1262.58	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	714.49	1.00
M052X M052X	AUG-cc-pVDZ	-1262.58	-1262.60	-1262.74	-1261.35	-1261.46	-1261.60	715.63	1.16
M052X	AUG-cc-pVTZ	-1262.58	-1262.64	-1262.75	-1261.35	-1261.46	-1261.61	713.84	0.91
M052X	AUG-cc-pVQZ	-1262.58	-1262.65	-1262.75	-1261.36	-1261.43	-1261.61	714.49	1.00
M052X M052X	SV SV	-1262.39	-1262.45	-1262.76	-1261.15	-1261.26	-1261.41	720.70	1.88
M052X M052X	SVP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.26	-1261.41	719.00	1.64
M052X	TZV	-1262.55	-1262.40	-1262.72	-1261.32	-1261.44	-1261.58	711.62	0.59
M052X M052X	TZVP	-1262.55	-1262.61	-1262.72	-1261.32	-1261.44	-1261.58	711.85	0.63
M052X M052X	QZVP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.47	-1261.61	714.43	0.99
M052X M052X	def2SV	-1262.39	-1262.46	-1262.76	-1261.15	-1261.26	-1261.42	719.00	1.64
M052X M052X	def2SVP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.27	-1261.42	719.60	1.72
M052X M052X	def2SVPP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.27	-1261.42	719.00	1.64
M052X M052X	def2TZV	-1262.55	-1262.40	-1262.72	-1261.13	-1261.44	-1261.42	713.60	0.59
M052X M052X	def2TZVP	-1262.55	-1262.61	-1262.72	-1261.33	-1261.44	-1261.58	711.02	0.69
M052X M052X	def2TZVPP	-1262.55	-1262.61	-1262.72	-1261.33	-1261.44	-1261.58	712.72	0.09
M052X M052X	def2QZV	-1262.58	-1262.64	-1262.72	-1261.35	-1261.44	-1261.58	713.29	0.73
M052X M052X	def2QZVP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.46	-1261.61	713.29	0.83
M052X M052X	def2QZVPP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.47	-1261.61	714.43	1.00
	ueizWZVFF			-1202.75					
PBE1PBE		-1248.65	-1248.86	-1240.98	-1247.85	-1247.92	-1248.10	554.92	21.56

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

PBEIPBE	D	Dania aut	1	3	_	2	4	C	3IE	07 E
PBEIPBE 6-31g(d,p)	Functional	Basis set	1		5		4	6		%Error
PBEIPBE 6-31+g(d,p) 1-262_26 1262_32 1-262_42 1-261_02 1-261_12 1-261_27 719_91 1.77 PBEIPBE 6-31+g(d,p) 1-262_66 1262_32 1-262_42 1-261_02 1-261_12 1-261_27 720_27 1.82 PBEIPBE 6-31+g(d,p) 1-262_66 1262_32 1-262_42 1-261_02 1-261_12 1-261_27 720_27 1.82 PBEIPBE 6-31+g(d,p) 1-262_66 1262_32 1-262_42 1-261_02 1-261_12 1-261_27 720_27 1.82 PBEIPBE ccpVDZ 1-262_42 1-262_48 1-262_58 1-261_18 1-261_28 1-261_44 719_38 1.69 PBEIPBE ccpVQZ 1-262_43 1-262_48 1-262_58 1-261_18 1-261_28 1-261_44 719_38 1.69 PBEIPBE AUG-ccpVDZ 1-262_43 1-262_44 1-262_58 1-261_18 1-261_28 1-261_44 719_38 1.69 PBEIPBE AUG-ccpVQZ 1-262_43 1-262_44 1-262_58 1-261_19 1-261_29 1-261_44 719_30 1.69 PBEIPBE AUG-ccpVQZ 1-262_42 1-262_48 1-262_59 1-261_19 1-261_29 1-261_44 719_30 1.69 PBEIPBE SV 1-262_42 1-262_48 1-262_59 1-261_19 1-261_29 1-261_44 719_30 1.69 PBEIPBE SV 1-262_43 1-262_49 1-262_59 1-261_19 1-261_29 1-261_44 719_30 1.69 PBEIPBE SV 1-262_43 1-262_49 1-262_59 1-261_19 1-261_29 1-261_44 719_30 1.69 PBEIPBE TZV 1-262_40 1-262_46 1-262_56 1-261_16 1-261_29 1-261_44 719_30 1.69 PBEIPBE TZV 1-262_40 1-262_46 1-262_56 1-261_16 1-261_26 1-261_44 717_39 1.47 PBEIPBE dcPSV 1-262_43 1-262_49 1-262_59 1-261_16 1-261_26 1-261_44 717_39 1.47 PBEIPBE dcPSV 1-262_23 1-262_29 1-262_39 1-260_39 1-260_19 1-261_29 1-261_44 719_67 1.73 PBEIPBE dcPSV 1-262_23 1-262_29 1-262_39 1-260_39 1-260_19 1-261_29 1-261_44 719_67 1.73 PBEIPBE dcPSV 1-262_40 1-262_56 1-261_19 1-261_29 1-261_44 7-265_70 2-70 PBEIPBE dcPSV 1-262_40 1-262_56 1-261_19 1-261_29 1-261_44 7-265_70 2-70 PBEIPBE dcPSV 1-262_40 1-262_56 1-261_19 1-261_29 1-261_44 7-265_70 2-70 PBEIPBE dcPSV 1-262_4										
PBEIPBE G-31++g 1-202.26 1262.32 1-202.42 1-201.02 1-201.12 1-201.27 79.97 1.82 PBEIPBE G-31++g 1-202.26 1262.32 1-202.42 1-201.02 1-201.12 1-201.27 79.99 1.77 PBEIPBE G-31++g 1-202.26 1262.32 1-202.42 1-201.02 1-201.12 1-201.27 79.97 1.82 PBEIPBE G-pVDZ 1-202.42 1-202.48 1-202.59 1-201.18 1-201.28 1-201.43 721.54 2.00 PBEIPBE C-pVDZ 1-202.42 1-202.48 1-202.59 1-201.18 1-201.29 1-201.44 719.78 1.79 PBEIPBE C-pVDZ 1-202.42 1-202.48 1-202.59 1-201.18 1-201.28 1-201.44 719.78 1.79 PBEIPBE AUG-c-pVDZ 1-202.42 1-202.44 1-202.58 1-201.18 1-201.28 1-201.44 719.79 1.75 PBEIPBE AUG-c-pVDZ 1-202.42 1-202.44 1-202.58 1-201.18 1-201.28 1-201.44 719.79 1.75 PBEIPBE AUG-c-pVDZ 1-202.42 1-202.44 1-202.59 1-201.19 1-201.29 1-201.44 719.79 1.75 PBEIPBE SV 1-202.23 1-202.39 1-202.39 1-201.19 1-201.29 1-201.44 719.79 1.75 PBEIPBE SV 1-202.23 1-202.39 1-202.39 1-200.98 1-201.80 1-201.81 1-2		6-31g(d,p)								
PBEIPBE										
PBEIPBE 6-31++g(d,p) -1262.26 -1262.32 -1262.42 -1261.02 -1261.12 -1261.27 720.27 1.82 PBEIPBE cc-pVDZ -1262.42 -1262.48 -1262.55 -1261.19 -1261.29 -1261.44 719.38 1.69 PBEIPBE cc-pVDZ -1262.42 -1262.48 -1262.55 -1261.19 -1261.29 -1261.44 719.38 1.69 PBEIPBE AUG-cc-pVDZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE AUG-cc-pVDZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE AUG-cc-pVDZ -1262.42 -1262.48 -1262.55 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE AUG-cc-pVDZ -1262.43 -1262.49 -1262.59 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.37 728.10 2.92 PBEIPBE SVP -1262.24 -1262.45 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE TZV -1262.40 -1262.45 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE QZVP -1262.44 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE de/2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.41 717.79 1.47 PBEIPBE de/2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.41 717.79 1.47 PBEIPBE de/2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.41 715.77 2.59 PBEIPBE de/2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2CV -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE de/2CV -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE de/2CV -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE de/2CV -1262.40 -1262.46 -1262.56 -1261.16 -1261.2		6-31+g(d,p)								
PBEIPBE Cc-pVIZ -1262.42 -1262.48 -1262.55 -1261.18 -1261.29 -1261.43 721.54 2.00 PBEIPBE Cc-pVIZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.38 1.69 PBEIPBE Cc-pVIZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE AUG-cc-pVIZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.70 1.69 PBEIPBE AUG-cc-pVIZ -1262.42 -1262.44 -1262.55 -1261.19 -1261.29 -1261.44 719.70 1.69 PBEIPBE SV -1262.43 -1262.49 -1262.55 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.34 719.79 1.75 PBEIPBE SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE TZV -1262.40 -1262.45 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE QZVP -1262.42 -1262.45 -1262.55 -1261.10 -1261.26 -1261.41 717.79 1.48 PBEIPBE QZVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2TVP -1262.23 -1262.29 -1262.40 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE de/2TVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 PBEIPBE de/2TVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 PBEIPBE de/2TVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 PBEIPBE de/2CVPP -1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.41 718.46 PBEIPBE de/2CVPP -1262.42 -1262.48 -1262.56 -1261.16 -1261.26 -1261.41 718.46 PBEIPBE de/										
PBEIPBE CC-PVTZ		6-31++g(d,p)								
PBEIPBE			-1262.42							
PBEIPBE AUG-cc-pVDZ -1262.42 -1262.44 -1262.55 -1261.18 -1261.28 -1261.43 721.41 1.98 PBEIPBE AUG-cc-pVDZ -1262.43 -1262.49 -1262.59 -1261.19 -1261.29 -1261.44 719.79 1.75 PBEIPBE SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.23 728.10 2.92 PBEIPBE SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.23 728.10 2.92 PBEIPBE SVP -1262.40 -1262.45 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE TZV -1262.40 -1262.45 -1262.56 -1261.16 -1261.26 -1261.41 717.79 1.47 PBEIPBE dc2VP -1262.40 -1262.48 -1262.59 -1261.16 -1261.26 -1261.41 717.92 1.48 PBEIPBE dc2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE dc2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 719.67 1.73 PBEIPBE dc2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.44 725.77 2.59 PBEIPBE dc2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.47 725.77 2.59 PBEIPBE dc2TZV -1262.30 -1262.36 -1262.56 -1261.16 -1261.26 -1261.41 717.79 -147 PBEIPBE dc2TZVP -1262.30 -1262.36 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE dc2TZVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE dc2TZVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.46 1.56 PBEIPBE dc2CZVP -1262.40 -1262.46 -1262.56 -1261.19 -1261.29 -1261.41 718.94 1.63 PBEIPBE dc2CZVP -1262.42 -1262.48 -1262.56 -1261.19 -1261.29 -1261.44 718.94 1.63 PBEIPBE dc2CZVP -1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.73 PBEIPBE dc2CZVP -1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.73 PBEIPBE dc2CZVP -1262.42 -1262.33 -1262.49 -1261.19 -1261.29 -1261.44 719.67 1.73 PBEIPBE dc2CZVP -1	PBE1PBE		-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.38	1.69
PBEIPBE AUG-cc-pVTZ 1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.44 719.40 1.69 PBEIPBE AUG-cc-pVQZ -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.23 728.10 2.92 PBEIPBE SV	PBE1PBE		-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	719.79	1.75
PBEIPBE SVP -1262.23 -1262.49 -1262.59 -1261.09 -1261.08 -1261.23 728.10 2.99 PBEIPBE SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE TZV -1262.40 -1262.40 -1262.65 -1261.61 -1261.26 -1261.41 717.79 1.47 PBEIPBE TZVP -1262.40 -1262.26 -1262.65 -1261.61 -1261.26 -1261.41 717.79 1.47 PBEIPBE CZVP -1262.42 -1262.48 -1262.55 -1261.61 -1261.29 -1261.41 717.79 1.47 PBEIPBE def2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.20 -1262.40 -1262.56 -1261.61 -1261.62 -1261.41 717.79 1.47 PBEIPBE def2TZVP -1262.40 -1262.46 -1262.56 -1261.61 -1261.26 -1261.41 718.46 1.56 PBEIPBE def2TZVP -1262.40 -1262.46 -1262.56 -1261.61 -1261.26 -1261.41 718.46 1.56 PBEIPBE def2ZVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.94 1.63 PBEIPBE def2ZVP -1262.42 -1262.48 -1262.56 -1261.16 -1261.26 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.55 -1261.18 -1261.29 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.18 -1261.29 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.18 -1261.29 -1261.44 719.67 1.73 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.73 PBEIPBE def2ZVPP -1262.42 -1262.38 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.74 HSEHIPBE def31.44 -1262.26 -1262.33 -1262.43 -1261.03 -1261.33 -1261.45 720.38 1.83 HSEHIPBE def3	PBE1PBE	AUG-cc-pVDZ	-1262.42	-1262.44	-1262.58	-1261.18	-1261.28	-1261.43	721.41	1.98
PBEIPBE SVP -1262.23 -1262.49 -1262.59 -1261.09 -1261.08 -1261.23 728.10 2.99 PBEIPBE SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE TZV -1262.40 -1262.40 -1262.65 -1261.61 -1261.26 -1261.41 717.79 1.47 PBEIPBE TZVP -1262.40 -1262.26 -1262.65 -1261.61 -1261.26 -1261.41 717.79 1.47 PBEIPBE CZVP -1262.42 -1262.48 -1262.55 -1261.61 -1261.29 -1261.41 717.79 1.47 PBEIPBE def2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SV -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.23 -1262.29 -1262.39 -1260.98 -1261.08 -1261.24 725.77 2.59 PBEIPBE def2SVP -1262.20 -1262.40 -1262.56 -1261.61 -1261.62 -1261.41 717.79 1.47 PBEIPBE def2TZVP -1262.40 -1262.46 -1262.56 -1261.61 -1261.26 -1261.41 718.46 1.56 PBEIPBE def2TZVP -1262.40 -1262.46 -1262.56 -1261.61 -1261.26 -1261.41 718.46 1.56 PBEIPBE def2ZVP -1262.40 -1262.46 -1262.56 -1261.16 -1261.26 -1261.41 718.94 1.63 PBEIPBE def2ZVP -1262.42 -1262.48 -1262.56 -1261.16 -1261.26 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.55 -1261.18 -1261.29 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.18 -1261.29 -1261.44 718.94 1.63 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.18 -1261.29 -1261.44 719.67 1.73 PBEIPBE def2ZVPP -1262.42 -1262.48 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.73 PBEIPBE def2ZVPP -1262.42 -1262.38 -1262.59 -1261.19 -1261.29 -1261.44 719.67 1.74 HSEHIPBE def31.44 -1262.26 -1262.33 -1262.43 -1261.03 -1261.33 -1261.45 720.38 1.83 HSEHIPBE def3	PBE1PBE	AUG-cc-pVTZ	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.40	1.69
PBEIPBE TZV	PBE1PBE		-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	719.79	1.75
PBEIPBE TZV	PBE1PBE	SV	-1262.23	-1262.29	-1262.39	-1260.98	-1261.08	-1261.23	728.10	2.92
PBEIPBE TZV		SVP				-1260.98		-1261.24	725.77	
PBEIPBE QZVP -1262.40 -1262.46 -1262.59 -1261.19 -1261.29 -1261.44 717.92 1.48							-1261.26			
PBEIPBE QZVP -1262.42 -1262.28 -1262.39 -1261.99 -1261.08 -1261.44 719.67 1.73										
PBEIPBE def2SV										
PBE1PBE def2SVP										
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HSEH1PBE cc-pVTZ										
HSEH1PBE Cc-pVQZ										
HSEH1PBE AUG-cc-pVDZ -1262.43 -1262.46 -1262.59 -1261.19 -1261.29 -1261.44 722.12 2.08 HSEH1PBE AUG-cc-pVTZ -1262.44 -1262.49 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.78 HSEH1PBE AUG-cc-pVQZ -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.38 1.83 HSEH1PBE SV -1262.24 -1262.26 -1262.40 -1260.99 -1261.09 -1261.24 728.63 3.00 HSEH1PBE SVP -1262.25 -1262.30 -1262.41 -1260.99 -1261.06 -1261.25 726.31 2.67 HSEH1PBE TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.48 1.56 HSEH1PBE TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.61 1.58 HSEH1PBE QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.82 HSEH1PBE def2SV -1262.25 -1262.30 -1262.41 -1260.99 -1261.10 -1261.25 726.31 2.67 HSEH1PBE def2SVP -1262.25 -1262.30 -1262.41 -1260.09 -1261.10 -1261.25 726.31 2.67 HSEH1PBE def2SVP -1262.25 -1262.30 -1262.41 -1260.09 -1261.10 -1261.25 727.04 2.77 HSEH1PBE def2SVP -1262.25 -1262.30 -1262.41 -1260.09 -1261.10 -1261.25 726.31 2.67 HSEH1PBE def2TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.48 1.56 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.14 1.66 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.14 1.66 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.14 1.66 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.62 1.72										
HSEH1PBE AUG-cc-pVTZ -1262.44 -1262.49 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.78 HSEH1PBE AUG-cc-pVQZ -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.38 1.83 HSEH1PBE SV -1262.24 -1262.26 -1262.40 -1260.99 -1261.09 -1261.24 728.63 3.00 HSEH1PBE SVP -1262.25 -1262.30 -1262.41 -1260.99 -1261.06 -1261.25 726.31 2.67 HSEH1PBE TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.48 1.56 HSEH1PBE TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.61 1.58 HSEH1PBE QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.82 HSEH1PBE def2SV -1262.25 -1262.30 -1262.41 -1260.99 -1261.10 -1261.25 726.31 2.67 HSEH1PBE def2SVP -1262.25 -1262.31 -1262.41 -1260.09 -1261.10 -1261.25 727.04 2.77 HSEH1PBE def2SVPP -1262.25 -1262.30 -1262.41 -1260.99 -1261.10 -1261.25 726.31 2.67 HSEH1PBE def2TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 718.48 1.56 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.44 1.66 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.14 1.66 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.62 1.72 HSEH1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.62 1.72										
HSEH1PBE AUG-cc-pVQZ -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.38 1.83 HSEH1PBE SV										
HSEH1PBE SV										
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$										
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			-1262.44						720.31	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$										2.67
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	HSEH1PBE	def2SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	727.04	2.77
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	HSEH1PBE	def2SVPP	-1262.25	-1262.30	-1262.41	-1260.99	-1261.10	-1261.25	726.31	2.67
HSEH1PBE def2TZVPP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.62 1.72	HSEH1PBE	def2TZV	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	718.48	1.56
HSEH1PBE def2TZVPP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.42 719.62 1.72	HSEH1PBE	def2TZVP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	719.14	1.66
				-1262.47						
	HSEH1PBE	def2QZV		-1262.49	-1262.60		-1261.30	-1261.45	718.98	1.63

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE	%Error
							_	Kcal/mol	
HSEH1PBE	def2QZVP	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.31	1.82
HSEH1PBE	def2QZVPP	-1262.44	-1262.46	-1262.60	-1261.20	-1261.30	-1261.45	720.39	1.83
OHSE2PBE OHSE2PBE	C 91	-1248.95	-1249.15	-1249.27	-1248.13	-1248.20	-1248.38	560.07	20.83
	6-31g	-1262.53	-1262.59	-1262.69	-1261.29	-1261.39 -1261.39	-1261.54	721.24	1.95
OHSE2PBE	6-31g(d,p)	-1262.53	-1262.59	-1262.69	-1261.29		-1261.54	721.61	2.01
OHSE2PBE	6-31+g	-1262.55	-1262.61	-1262.71	-1261.30	-1261.40	-1261.55	727.27	2.81
OHSE2PBE	6-31+g(d,p)	-1262.55	-1262.61	-1262.71	-1261.30	-1261.40	-1261.55	727.62	2.86
OHSE2PBE	6-31++g	-1262.55	-1262.61	-1262.71	-1261.30	-1261.40	-1261.55	727.27	2.81
OHSE2PBE	6-31++g(d,p)	-1262.55	-1262.61	-1262.71	-1261.30	-1261.40	-1261.55	727.62	2.86
OHSE2PBE	cc-pVDZ	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	729.01	3.05
OHSE2PBE	cc-pVTZ	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	726.78	2.74
OHSE2PBE	cc-pVQZ	-1262.71	-1262.77	-1262.87	-1261.47	-1261.57	-1261.72	727.13	2.79
OHSE2PBE	AUG-cc-pVDZ	-1262.71	-1262.73	-1262.87	-1261.46	-1261.56	-1261.71	728.88	3.03
OHSE2PBE	AUG-cc-pVTZ	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	726.80	2.74
OHSE2PBE	AUG-cc-pVQZ	-1262.71	-1262.77	-1262.87	-1261.47	-1261.57	-1261.72	727.13	2.79
OHSE2PBE	SV	-1262.52	-1262.58	-1262.68	-1261.25	-1261.35	-1261.51	735.48	3.97
OHSE2PBE	SVP	-1262.52	-1262.58	-1262.68	-1261.26	-1261.36	-1261.51	733.15	3.64
OHSE2PBE	TZV	-1262.68	-1262.74	-1262.84	-1261.44	-1261.54	-1261.69	725.23	2.52
OHSE2PBE	TZVP	-1262.68	-1262.74	-1262.84	-1261.44	-1261.54	-1261.69	725.36	2.54
OHSE2PBE	QZVP	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	727.06	2.78
OHSE2PBE	def2SV	-1262.52	-1262.58	-1262.68	-1261.26	-1261.36	-1261.51	733.15	3.64
OHSE2PBE	def2SVP	-1262.52	-1262.58	-1262.68	-1261.26	-1261.36	-1261.51	733.87	3.74
OHSE2PBE	def2SVPP	-1262.52	-1262.58	-1262.68	-1261.26	-1261.36	-1261.51	733.15	3.64
OHSE2PBE	def2TZV	-1262.68	-1262.74	-1262.84	-1261.44	-1261.54	-1261.69	725.23	2.52
OHSE2PBE	def2TZVP	-1262.68	-1262.74	-1262.85	-1261.44	-1261.54	-1261.69	725.88	2.61
OHSE2PBE	def2TZVPP	-1262.68	-1262.74	-1262.85	-1261.44	-1261.54	-1261.69	726.36	2.68
OHSE2PBE	def2QZV	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	725.73	2.59
OHSE2PBE	def2QZVP	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	727.06	2.78
OHSE2PBE	def2QZVPP	-1262.71	-1262.77	-1262.87	-1261.46	-1261.56	-1261.71	727.15	2.79
B98		-1248.39	-1248.91	-1249.11	-1248.00	-1248.11	-1248.22	554.41	21.63
B98	6-31g	-1262.44	-1262.39	-1262.58	-1261.24	-1261.30	-1261.44	717.41	1.41
B98	6-31g(d,p)	-1262.44	-1262.39	-1262.58	-1261.24	-1261.30	-1261.44	717.70	1.45
B98	6-31+g	-1262.46	-1262.50	-1262.60	-1261.22	-1261.34	-1261.44	723.97	2.34
B98	6-31+g(d,p)	-1262.46	-1262.50	-1262.60	-1261.22	-1261.34	-1261.44	724.24	2.38
B98	6-31++g	-1262.46	-1262.50	-1262.60	-1261.22	-1261.26	-1261.44	723.97	2.34
B98	6-31++g(d,p)	-1262.46	-1262.50	-1262.60	-1261.22	-1261.34	-1261.44	724.24	2.38
B98	cc-pVDZ	-1262.62	-1262.66	-1262.76	-1261.38	-1261.50	-1261.61	724.09	2.36
B98	cc-pVTZ	-1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	722.53	2.14
B98	cc-pVQZ	-1262.62	-1262.67	-1262.77	-1261.39	-1261.51	-1261.61	723.15	2.22
B98	AUG-cc-pVDZ	-1262.62	-1262.66	-1262.76	-1261.38	-1261.42	-1261.61	724.32	2.39
B98	AUG-cc-pVTZ	-1262.62	-1262.66	-1262.76	-1261.39	-1261.43	-1261.61	722.83	2.18
B98	AUG-cc-pVQZ	-1262.62	-1262.67	-1262.77	-1261.39	-1261.44	-1261.61	723.44	2.26
B98	SV	-1262.43	-1262.47	-1262.57	-1261.18	-1261.30	-1261.40	730.72	3.29
B98	SVP	-1262.43	-1262.47	-1262.57	-1261.18	-1261.30	-1261.41	728.59	2.99
B98	TZV	-1262.59	-1262.63	-1262.73	-1261.36	-1261.40	-1261.58	721.27	1.96
B98	TZVP	-1262.59	-1262.63	-1262.73	-1261.36	-1261.48	-1261.58	721.44	1.98
B98	QZVP	-1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	722.88	2.19
B98	def2SV	-1262.43	-1262.47	-1262.57	-1261.18	-1261.30	-1261.41	728.59	2.99
B98	def2SVP	-1262.43	-1262.47	-1262.57	-1261.18	-1261.31	-1261.41	728.90	3.04
B98	def2SVPP	-1262.43	-1262.47	-1262.57	-1261.18	-1261.30	-1261.41	728.26	2.95
B98	def2TZV	-1262.59	-1262.63	-1262.73	-1261.36	-1261.48	-1261.58	720.95	1.91

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE	%Error
B98	def2TZVP	-1262.59	-1262.63	-1262.74	-1261.36	-1261.48	-1261.58	Kcal/mol 721.92	2.05
B98	def2TZVPP	-1262.59	-1262.63	-1262.74	-1261.36	-1261.48	-1261.58	721.92	2.05
B98	def2QZV	-1262.69	-1262.66	-1262.74	-1261.39	-1261.48	-1261.69	722.34	2.11
B98	def2QZVP		-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	723.17	2.00
B98	def2QZVPP	-1262.62 -1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	723.17	2.23
B972	deizQZVFF	-1202.02	-1202.00	-1202.70	-1201.39	-1248.44	-1201.01	550.22	22.22
B972 B972	6-31g	-1249.14	-1249.25	-1249.46	-1248.32	-1248.44	-1248.58	715.34	1.12
B972	6-31g(d,p)		-1262.77		-1261.49	-1261.62	-1261.74	715.54	1.12
B972	6-31+g	-1262.72 -1262.74	-1262.77	-1262.88 -1262.89	-1261.49	-1261.62	-1261.74	715.01	1.10
B972	6-31+g 6-31+g(d,p)	-1262.74	-1262.78	-1262.89	-1261.50	-1261.63	-1261.74	721.00	1.93
B972	6-31+g(d,p) 6-31++g	-1262.74	-1262.78	-1262.89	-1261.50	-1261.63	-1261.74	721.33	1.97
B972	6-31++g 6-31++g(d,p)	-1262.74	-1262.78	-1262.89	-1261.50	-1261.55	-1261.74	721.00	1.93
	cc-pVDZ								
B972 B972	cc-pVTZ	-1262.90	-1262.95	-1263.05	-1261.66	-1261.79 -1261.72	-1261.90	721.86	2.04 1.72
B972 B972	cc-pV1Z cc-pVQZ	-1262.90	-1262.95	-1263.06 -1263.06	-1261.67 -1261.67		-1261.91 -1261.91	719.61 720.53	1.72
		-1262.91	-1262.95			-1261.72			
B972 B972	AUG-cc-pVDZ	-1262.90	-1262.95	-1263.05	-1261.66	-1261.71	-1261.90 -1261.91	722.01	2.06
B972 B972	AUG-cc-pVTZ AUG-cc-pVQZ	-1262.90	-1262.95	-1263.06 -1263.06	-1261.67 -1261.67	-1261.72 -1261.72	-1261.91	719.62	1.73 1.83
B972	SV	-1262.91 -1262.71	-1262.95 -1262.75	-1262.86	-1261.67	-1261.72	-1261.91	720.37 728.59	2.99
B972	SVP	-1262.71	-1262.76	-1262.87	-1261.46	-1261.59	-1261.70	726.05	2.63
B972	TZV			-1263.03	-1261.46	-1261.77	-1261.71	718.48	1.56
B972	TZVP	-1262.88 -1262.88	-1262.92 -1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.62	1.58
B972 B972	QZVP	-1262.90	-1262.95	-1263.06 -1262.86	-1261.67 -1261.46	-1261.72	-1261.91	719.97	1.77
	def2SV def2SVP	-1262.71	-1262.76		-1261.46	-1261.51	-1261.71 -1261.71	725.78	2.60 2.68
B972		-1262.71	-1262.76	-1262.87		-1261.59		726.40	
B972 B972	def2SVPP def2TZV	-1262.71 -1262.88	-1262.76 -1262.92	-1262.86 -1263.03	-1261.46 -1261.64	-1261.51 -1261.77	-1261.71 -1261.88	725.78 718.23	2.60 1.53
B972 B972	def2TZVP	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.23	1.62
B972	def2TZVPP	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	719.51	1.71
B972	def2QZV	-1262.90	-1262.92		-1261.64	-1261.77	-1261.88	719.09	1.65
B972	def2QZVP	-1262.90	-1262.95	-1263.06 -1263.06	-1261.67	-1261.79	-1261.91	719.09	1.80
B972 B972	def2QZVPP			-1263.06	-1261.67	-1261.80	-1261.91	720.19	1.80
OHSE1PBE	deizQZVFF	-1262.90	-1262.95						
OHSE1PBE OHSE1PBE	6-31g	-1248.67 -1262.26	-1248.88 -1262.32	-1249.00 -1262.42	-1247.87 -1261.03	-1247.90 -1261.13	-1248.12 -1261.28	554.89 714.36	21.56 0.98
OHSE1PBE OHSE1PBE	6-31g(d,p)	-1262.26	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	714.50	1.03
	6-31+g	-1262.27	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	720.53	1.05
OHSE1PBE OHSE1PBE	6-31+g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.88	1.90
OHSE1PBE OHSE1PBE	6-31+g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.53	1.85
							-1261.28		
OHSE1PBE OHSE1PBE	6-31++g(d,p) cc-pVDZ	-1262.27 -1262.43	-1262.33 -1262.46	-1262.43 -1262.60	-1261.03 -1261.19	-1261.13 -1261.29	-1261.28 -1261.44	720.88 722.26	1.90 2.10
			-1262.40			-1261.29		720.03	
OHSE1PBE OHSE1PBE	cc-pVTZ cc-pVQZ	-1262.44 -1262.44	-1262.50	-1262.60 -1262.60	-1261.20 -1261.20	-1261.30	-1261.45 -1261.45	720.03	1.78 1.83
OHSE1PBE OHSE1PBE									2.08
	AUG-cc-pVDZ AUG-cc-pVTZ	-1262.43	-1262.46	-1262.60	-1261.19	-1261.29	-1261.44 -1261.45	722.13 720.05	
OHSE1PBE OHSE1PBE	AUG-cc-pV1Z AUG-cc-pVQZ	-1262.44 -1262.44	-1262.50 -1262.50	-1262.60 -1262.60	-1261.20 -1261.20	-1261.30 -1261.30	-1261.45	720.05	1.79 1.83
OHSE1PBE OHSE1PBE	SV	-1262.44	-1262.30	-1262.41	-1261.20	-1261.30	-1261.45	720.39	3.00
OHSE1PBE OHSE1PBE	SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.09	-1261.24	726.34	2.67
OHSE1PBE	TZV	-1262.23	-1262.47	-1262.41	-1261.00	-1261.10	-1261.23	718.49	1.56
OHSE1PBE OHSE1PBE	TZVP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	718.49	1.58
OHSE1PBE OHSE1PBE	QZVP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	720.32	1.58
OHSE1PBE OHSE1PBE	def2SV		-1262.31			-1261.30			
OUSFILDE	ue125 V	-1262.25	-1202.31	-1262.41	-1261.00	-1201.00	-1261.25	726.34	2.67

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

OHSEIPBE def2SVPP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.04 2.67	Functional	Basis set	1	3	5	2	4	6	3IE	%Error
OHSEIPBE dePTZV 1-262.41 1262.47 1262.47 1262.57 1261.17 1261.27 1261.43 1791.4 1.66 OHSEIPBE dePTZVP 1262.41 1262.47 1262.57 1261.17 1261.27 1261.43 1791.4 1.66 OHSEIPBE dePZZVP 1262.41 1262.47 1262.57 1261.18 1261.27 1261.43 1791.4 1.66 OHSEIPBE dePZZVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.43 1791.4 1.66 OHSEIPBE dePZZVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 OHSEIPBE dePZZVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 OHSEIPBE dePZZVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 OHSEIPBE dePZZVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 OHSEIPBE dePZZVPP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 PBENIPBE dePZZVPP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 1781.89 1.64 PBENIPBE 6-31g 1262.26 1262.32 1262.42 1261.03 1261.30 1261.45 1701.40 1881.89 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 1705.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 1705.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBENIPBE 6-31Hg 1262.27 1262.33 1262.44 1261.00 1261.03 1261.13 1261.29 720.55 1.86 PBENIPBE CPVDZ 1262.44 1262.46 1262.60 1261.20 1261.30 1261.45 720.04 1.88 PBENIPBE AUG-ce-pVDZ 1262.44 1262.60 1262.00 1261.20 1261.30 1261.45 720.04 1.88 PBENIPBE AUG-ce-pVDZ 1262.44 1262.60 1262.00 1261.20 1261.30 1261.45 720.04 1.89 PBENIPBE AUG-ce-pVDZ					_			_	Kcal/mol	
OHSEIPBE defTZVP 1-262.41 1262.47 1-262.57 1-261.17 1-261.27 1261.42 718.94 1.56 OHSEIPBE defTZVP 1-262.41 1262.47 1-262.57 1-261.17 1261.27 1261.43 719.63 1.73 OHSEIPBE defZZVP 1-262.41 1-262.47 1-262.57 1-261.18 1-261.27 1261.43 719.63 1.73 OHSEIPBE defZZVP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.27 1-261.45 718.99 1.64 OHSEIPBE defZZVP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.27 1-261.45 718.99 1.64 OHSEIPBE defZZVP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.27 1-261.45 718.99 1.64 OHSEIPBE defZZVPP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.27 1-261.45 720.32 1.82 OHSEIPBE defZZVPP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.30 1-261.45 720.32 1.82 OHSEIPBE defZZVPP 1-262.44 1-262.50 1-262.60 1-261.20 1-261.30 1-261.45 720.32 1.82 PBEHIPBE 6-31g 1-262.27 1-262.33 1-240.42 1-261.03 1-261.13 1-261.28 714.35 0.99 PBEHIPBE 6-31g(d,p) 1-262.26 1-262.32 1-262.42 1-261.03 1-261.03 1-261.33 1-261.28 714.37 0.99 PBEHIPBE 6-31g(d,p) 1-262.27 1-262.33 1-262.43 1-261.03 1-261.13 1-261.29 720.55 1.86 PBEHIPBE 6-31g(d,p) 1-262.27 1-262.33 1-262.43 1-261.03 1-261.13 1-261.29 720.55 1.86 PBEHIPBE 6-31g(d,p) 1-262.27 1-262.33 1-262.43 1-261.03 1-261.13 1-261.29 720.99 1.99 PBEHIPBE 6-31g(d,p) 1-262.27 1-262.33 1-262.43 1-261.03 1-261.13 1-261.29 720.99 1.99 PBEHIPBE cc-pVDZ 1-262.44 1262.46 1-262.60 1-261.19 1-261.19 1-261.29 1-261.45 722.27 2.10 PBEHIPBE C-pVDZ 1-262.44 1262.46 1-262.60 1-261.19 1-261.13 1-261.29 720.99 1.99 PBEHIPBE NUG-cc-pVDZ 1-262.44 1-262.46 1-262.60 1-261.20 1-261.13 1-261.29 1-261.45 722.47 2.10 PBEHIPBE AUG-cc-pVDZ 1-262.44 1-262.46 1-262.60 1-261.20 1-261.13 1-261.45 720.40 1.83 PBEHIPBE AUG-cc-pVDZ 1-262.44 1-262.46 1-262.60 1-261.20 1-261.30 1-261.45 720.40 1.83 PBEHIPBE AUG-cc-pVDZ 1-262.44 1-262.46 1-262.60 1-261.20 1-261.20 1-261.30 1-261.45 720.40 1.83 PBEHIPBE AUG-cc-pVDZ 1-262.44 1-262.50 1-262.60 1-261.20 1-261.30 1-261.45 720.40 1.83 PBEHIPBE AUG-cc-pVDZ 1-262.44 1-262.60 1-262.00 1-261.20 1-261.30 1-261.45 720.40 1.83 PBEHIPBE CDA UG-cc-pVDZ 1-262.44 1-262.60 1-262.31 1-261.20 1-261.20 1										
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OIISEIPBE def2QXVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.35 718.99 1.64 OHSEIPBE def2QXVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.30 1.84 OHSEIPBE def2QXVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.30 1.84 OHSEIPBE def2QXVP 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.30 1.84 DHSEIPBE 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.40 1.84 DHSEIPBE 1262.44 1262.50 1262.60 1261.30 1261.35 1261.28 714.35 0.88 PBEHIPBE 6.31g(d.p.) 1262.26 1262.32 1262.42 1261.03 1261.13 1261.28 714.35 0.88 PBEHIPBE 6.31g(d.p.) 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBEHIPBE 6.31g(d.p.) 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBEHIPBE 6.31+g(d.p.) 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBEHIPBE 6.31+g(d.p.) 1262.27 1262.33 1262.43 1261.03 1261.13 1261.29 720.55 1.86 PBEHIPBE 6.31+g(d.p.) 1262.27 1262.33 1262.43 1261.03 1261.13 1261.99 720.90 1.90 PBEHIPBE 6.31+g(d.p.) 1262.27 1262.34 1262.60 1261.03 1261.13 1261.99 720.90 1.90 PBEHIPBE 6.31+g(d.p.) 1262.24 1262.46 1262.60 1261.03 1261.13 1261.29 720.55 1.86 PBEHIPBE 6.31+g(d.p.) 1262.24 1262.46 1262.60 1261.09 1261.30 1261.45 722.27 2.10 PBEHIPBE 6.31+g(d.p.) 1262.44 1262.46 1262.60 1261.09 1261.30 1261.45 722.27 2.10 PBEHIPBE 6.31+g(d.p.) 1262.24 1262.46 1262.60 1261.10 1261.30 1261.45 722.27 2.10 PBEHIPBE 700 1262.44 1262.46 1262.60 1261.10 1261.30 1261.45 720.04 1.83 PBEHIPBE AUG-cc-pVIZ 1262.44 1262.46 1262.60 1261.20 1261.30 1261.45 720.04 1.83 PBEHIPBE AUG-cc-pVIZ 1262.44 1262.46 1262.60 1261.20 1261.30 1261.45 720.04 1.83 PBEHIPBE 8V 1262.25 1262.31 1262.41 1261.00 1261.00 1261.35 726.33 2.67 PBEHIPBE 8V 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.06 1.79 PBEHIPBE 8V 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.06 1.79 PBEHIPBE 6422VP 1262.44 1262.50 1262.31 1262.41 1261.00 1261.00 1261.35 726.33 2.67 PBEHIPBE 6422VP 1262.44 1262.50 1262.50 1261.00 1261.00 1261.05 726.33 2.67 PBEHIPBE 6422VP 1262.44 1262.50 1262.31 1262.41 1261.00 1261.00 1261.45 720.00 1.83 P										
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PBEhIPBE		def2QZVPP								
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PBEhIPBE 6-31+g(d,p) -1262.27 -1262.33 -1262.43 -1261.03 -1261.13 -1261.29 720.55 1.86 PBEhIPBE 6-31+g(d,p) -1262.27 -1262.33 -1262.43 -1261.03 -1261.13 -1261.29 720.55 1.86 PBEhIPBE 6-31+g(d,p) -1262.27 -1262.33 -1262.43 -1261.03 -1261.13 -1261.29 720.55 1.86 PBEHIPBE 6-31+g(d,p) -1262.27 -1262.33 -1262.43 -1261.03 -1261.13 -1261.29 720.90 1.90 PBEHIPBE cc-pVDZ -1262.44 -1262.26 -1262.60 -1261.9 -1261.93 -1261.45 722.27 2.10 PBEHIPBE cc-pVDZ -1262.44 -1262.26 -1262.60 -1261.9 -1261.30 -1261.45 720.04 1.78 PBEHIPBE AUG-cc-pVDZ -1262.44 -1262.26 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.78 PBEHIPBE AUG-cc-pVDZ -1262.44 -1262.26 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.83 PBEHIPBE AUG-cc-pVZ -1262.44 -1262.26 -1262.60 -1261.20 -1261.30 -1261.45 720.06 1.79 PBEHIPBE AUG-cc-pVZ -1262.44 -1262.26 -1262.60 -1261.20 -1261.30 -1261.45 720.06 1.79 PBEHIPBE SV -1262.25 -1262.31 -1262.41 -1260.99 -1261.09 -1261.45 720.40 1.83 PBEHIPBE TZV -1262.25 -1262.31 -1262.41 -1260.99 -1261.09 -1261.25 726.33 2.67 PBEHIPBE TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.07 -1261.35 726.33 2.67 PBEHIPBE QZVP -1262.44 -1262.40 -1262.60 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE def2SV -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE def2SV -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.35 726.33 2.67 PBEHIPBE def2SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE def2SVP -1262.25 -1262.31 -1262.57 -1261.17 -1261.27 -1261.43 719.63 1.73 PBEHIPBE def2SVP -1262.44 -1262.50 -1262.57 -1261.18 -1261.30 -1261.45 720.33 1.66 PBEHIPBE def2SVP -1262.44 -1262.5										
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PBEINIPBE 6-31++g (Jp) -1262.27 -1262.33 -1262.43 -1261.03 -1261.13 -1261.29 720.55 1.86 PBENIPBE 6-31++g (Jp) -1262.24 -1262.33 -1262.45 -1261.03 -1261.19 -1261.45 720.27 2.10 PBENIPBE ccpVTZ -1262.44 -1262.46 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.78 PBENIPBE ccpVQZ -1262.44 -1262.50 -1260.60 -1261.20 -1261.30 -1261.45 720.04 1.83 PBENIPBE AUG-ccpVTZ -1262.44 -1262.60 -1261.20 -1261.30 -1261.45 720.06 1.79 PBENIPBE AUG-ccpVTZ -1262.44 -1262.46 -1262.60 -1261.20 -1261.35 720.06 1.79 PBENIPBE AUG-ccpVTZ -1262.44 -1262.46 -1262.60 -1261.20 -1261.45 720.06 1.79 PBENIPBE AUG-ccpVZV -1262.24 -1262.31 -1262.41 -1261.20 -1261.25		6-31+g								
PBEhIPBE Cc-pVDZ		6-31+g(d,p)								
PBEh1PBE cc-pVDZ -1262.44 -1262.46 -1262.60 -1261.20 -1261.30 -1261.45 722.27 2.10		6-31++g								
PBEh1PBE cc-pVTZ -1262.44 -1262.60 -1262.60 -1261.20 -1261.30 -1261.45 720.04 1.78		6-31++g(d,p)								
PBEh1PBE Cc-pVQZ 1262.44 1262.50 1262.60 1261.20 1261.30 1261.45 720.40 1.83		cc-pVDZ								
PBEh1PBE AUG-cc-pVDZ -1262.44 -1262.46 -1262.60 -1261.20 -1261.29 -1261.45 722.14 2.08										
PBEh1PBE AUG-cc-pVTZ -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.06 1.79 PBEh1PBE SUP -1262.25 -1262.31 -1262.41 -1260.90 -1261.30 -1261.25 728.64 3.00 PBEh1PBE SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.00 -1261.25 728.64 3.00 PBEh1PBE TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.49 1.56 PBEh1PBE TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.62 1.58 PBEh1PBE QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2SV -1262.25 -1262.31 -1262.41 -1261.00 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEh1PBE def2SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEh1PBE def2SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEh1PBE def2SVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEh1PBE def2TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.49 1.56 PBEh1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 719.15 1.66 PBEh1PBE def2QZVP -1262.41 -1262.47 -1262.57 -1261.18 -1261.28 -1261.43 719.15 1.66 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.43 719.63 1.73 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEB1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1	PBEh1PBE					-1261.20				
PBEhIPBE AUG-cc-pVQZ -1262.44 -1262.50 -1262.61 -1261.20 -1261.30 -1261.45 720.40 1.83 PBEhIPBE SV -1262.25 -1262.31 -1262.41 -1260.09 -1261.09 -1261.25 728.64 3.00 PBEhIPBE SVP -1262.45 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.49 1.56 PBEHIPBE TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.49 1.56 PBEHIPBE TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.62 1.58 PBEHIPBE DZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEHIPBE DZVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE DZVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE DZVP -1262.25 -1262.31 -1262.41 -1261.00 -1261.10 -1261.25 726.33 2.67 PBEHIPBE DZVP -1262.41 -1262.31 -1262.41 -1261.00 -1261.06 -1261.25 726.33 2.67 PBEHIPBE DZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 719.15 1.66 PBEHIPBE DZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 719.15 1.66 PBEHIPBE DZZVP -1262.41 -1262.47 -1262.57 -1261.18 -1261.25 -1261.43 719.15 1.66 PBEHIPBE DZZVP -1262.44 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEHIPBE DZZVP -1262.44 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEHIPBE DZZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEHIPBE DZZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.84 PBEHIPBE DZZZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.84 PBEHIPBE DZZZZP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.84 PBEHIPBE DZZZZP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.31 1.84 PBEHIPBE D										
PBEhIPBE SVP										
PBEh1PBE	PBEh1PBE	AUG-cc-pVQZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.40	
PBEh1PBE TZV						-1260.99				
PBEh1PBE										
PBEh1PBE QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82	PBEh1PBE		-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.43		1.56
PBEh1PBE def2SV	PBEh1PBE		-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.43		1.58
PBEh1PBE def2SVP					-1262.60	-1261.20		-1261.45	720.32	
PBEh1PBE def2SVPP	PBEh1PBE		-1262.25	-1262.31	-1262.41	-1261.00		-1261.25		
PBEh1PBE def2TZV -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 718.49 1.56 PBEh1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 719.15 1.66 PBEh1PBE def2TZVP -1262.44 -1262.47 -1262.57 -1261.18 -1261.28 -1261.43 719.63 1.73 PBEh1PBE def2QZV -1262.44 -1262.50 -1262.60 -1261.30 -1261.45 718.99 1.64 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVPP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.41 1.84 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.30	PBEh1PBE		-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	727.05	
PBEh1PBE def2TZVP -1262.41 -1262.47 -1262.57 -1261.17 -1261.27 -1261.43 719.15 1.66 PBEh1PBE def2TZVPP -1262.41 -1262.47 -1262.57 -1261.18 -1261.28 -1261.43 719.63 1.73 PBEh1PBE def2QZV -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 718.99 1.64 PBEh1PBE def2QZVP -1262.44 -1262.46 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVPP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVPP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.41 1.84 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.30 -1261.45 720.41 1.84 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.43	PBEh1PBE					-1261.00		-1261.25	726.33	
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PBEh1PBE def2QZV -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 718.99 1.64 PBEh1PBE def2QZVP -1262.44 -1262.46 -1262.60 -1261.20 -1261.30 -1261.45 720.32 1.82 PBEh1PBE def2QZVPP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.41 1.84 B1B95 -1249.05 -1249.25 -1249.37 -1248.24 -1248.26 -1248.48 553.87 21.71 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.43 -1261.53 -1261.67 714.79 1.04 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.43 -1261.53 -1261.67 714.79 1.04 B1B95 6-31g -1194.98 -1260.66 -1262.81 -1261.43 -1261.57 -1261.67 715.12 1.09 B1B95 6-31+g(d,p) -1232.86 -1260.39 -1262.83 -1222.1 -12										
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PBEh1PBE def2QZVPP -1262.44 -1262.50 -1262.60 -1261.20 -1261.30 -1261.45 720.41 1.84 B1B95 -1249.05 -1249.25 -1249.37 -1248.24 -1248.26 -1248.48 553.87 21.71 B1B95 6-31g -1262.66 -1262.72 -1262.81 -1261.43 -1261.53 -1261.67 714.79 1.04 B1B95 6-31g(d,p) -1262.66 -1262.72 -1262.81 -1261.43 -1261.53 -1261.67 715.12 1.09 B1B95 6-31+g -1194.98 -1260.66 -1262.83 -1261.52 -1261.57 -1261.68 720.73 1.88 B1B95 6-31+g(d,p) -1232.86 -1260.39 -1262.83 -1222.21 -1261.57 -1261.68 721.05 1.93 B1B95 6-31+g(d,p) -1232.86 -1260.66 -1262.83 -1222.21 -1261.57 -1261.68 721.05 1.93 B1B95 6-31+g(d,p) -1232.86 -1260.66 -1262.83 -1222.19										
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B1B95 6-31g(d,p) -1262.66 -1262.72 -1262.81 -1261.43 -1261.53 -1261.67 715.12 1.09 B1B95 6-31+g -1194.98 -1260.66 -1262.83 -1261.52 -1261.57 -1261.68 720.73 1.88 B1B95 6-31+g(d,p) -1232.86 -1260.39 -1262.83 -1222.21 -1261.57 -1261.68 721.05 1.93 B1B95 6-31++g -1262.68 -1260.66 -1262.83 -1222.19 -1261.57 -1261.68 720.73 1.88 B1B95 6-31++g(d,p) -1232.86 -1260.66 -1262.83 -1222.19 -1261.57 -1261.68 720.73 1.88 B1B95 6-31++g(d,p) -1232.86 -1260.24 -1262.83 -1222.19 -1261.57 -1261.68 720.73 1.88 B1B95 cc-pVDZ -1262.84 -1262.85 -1249.66 -1261.60 -1249.72 -1248.46 789.01 11.53 B1B95 cc-pVQZ -1262.84 -1262.99 -1261.60 <										
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	B1B95			-1256.24	-1262.83	-1222.21		-1261.68	721.05	
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B1B95 AUG-cc-pVQZ -1262.84 -1262.92 -1263.00 -1261.61 -1261.70 -1261.85 719.74 1.74 B1B95 SV -1262.65 -1262.70 -1262.80 -1261.39 -1261.49 -1261.64 728.63 3.00 B1B95 SVP -1262.65 -1262.70 -1262.80 -1261.40 -1261.50 -1261.64 726.25 2.66									787.87	11.37
B1B95 SV -1262.65 -1262.70 -1262.80 -1261.39 -1261.49 -1261.64 728.63 3.00 B1B95 SVP -1262.65 -1262.70 -1262.80 -1261.40 -1261.50 -1261.64 726.25 2.66	B1B95	AUG-cc-pVTZ		-1262.90		-1261.69			719.34	1.69
B1B95 SVP -1262.65 -1262.70 -1262.80 -1261.40 -1261.50 -1261.64 726.25 2.66		1 0								1.74
	B1B95		-1262.65			-1261.39		-1261.64	728.63	3.00
B1B95 TZV -1262.81 -1262.87 -1262.96 -1261.57 -1261.67 -1261.82 717.79 1.47				-1262.70						2.66
	B1B95	TZV	-1262.81	-1262.87	-1262.96	-1261.57	-1261.67	-1261.82	717.79	1.47

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
B1B95	TZVP	-1262.81	-1262.87	-1262.96	-1261.57	-1261.67	-1261.82	717.94	1.49
B1B95	QZVP	-1262.84	-1262.91	-1262.99	-1261.60	-1261.70	-1261.85	719.73	1.74
B1B95	def2SV	-1262.65	-1262.70	-1262.80	-1261.40	-1261.50	-1261.64	726.25	2.66
B1B95	def2SVP	-1262.65	-1262.70	-1262.80	-1261.40	-1261.50	-1261.64	726.88	2.75
B1B95	def2SVPP	-1262.65	-1262.70	-1262.80	-1261.40	-1261.50	-1261.64	726.25	2.66
B1B95	def2TZV	-1262.81	-1262.87	-1262.96	-1261.57	-1261.67	-1261.82	717.79	1.47
B1B95	def2TZVP	-1262.81	-1262.87	-1262.96	-1261.58	-1261.67	-1261.82	718.36	1.55
B1B95	def2TZVPP	-1262.81	-1262.87	-1262.97	-1261.58	-1261.67	-1261.82	718.77	1.60
B1B95	def2QZV	-1262.84	-1262.92	-1262.99	-1261.60	-1259.90	-1261.85	718.30	1.54
B1B95	def2QZVP	-1262.84	-1262.93	-1262.99	-1261.60	-1261.70	-1261.85	719.73	1.74
B1B95	def2QZVPP	-1262.84	-1262.93	-1262.99	-1261.60	-1261.70	-1261.85	719.81	1.75
TPSSh	doi2 Q2 (11	-1248.80	-1249.09	-1249.19	-1248.09	-1248.21	-1248.31	552.14	21.95
TPSSh	6-31g	-1262.49	-1262.54	-1262.64	-1261.26	-1261.36	-1261.49	717.56	1.43
TPSSh	6-31g(d,p)	-1262.49	-1262.54	-1262.64	-1261.27	-1261.36	-1261.49	717.94	1.49
TPSSh	6-31+g	-1262.51	-1262.56	-1262.65	-1261.27	-1261.36	-1261.50	724.49	2.41
TPSSh	6-31+g(d,p)	-1262.51	-1262.56	-1262.66	-1261.27	-1261.36	-1261.50	724.86	2.46
TPSSh	6-31++g	-1262.51	-1262.56	-1262.65	-1261.27	-1261.36	-1261.50	724.49	2.41
TPSSh	6-31++g(d,p)	-1262.51	-1262.56	-1262.66	-1261.27	-1261.36	-1261.50	724.86	2.46
TPSSh	cc-pVDZ	-1262.67	-1262.69	-1262.82	-1261.43	-1261.52	-1261.66	726.01	2.63
TPSSh	cc-pVTZ	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.17	2.37
TPSSh	cc-pV1Z	-1262.68	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.67	2.44
TPSSh	AUG-cc-pVDZ	-1262.67	-1262.72	-1262.82	-1261.43	-1261.52	-1261.66	725.90	2.61
TPSSh	AUG-cc-pVTZ	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.20	2.37
TPSSh	AUG-cc-pVQZ	-1262.68	-1262.73	-1262.82	-1261.44	-1261.58	-1261.67	724.20	2.44
TPSSh	SV	-1262.48	-1262.73	-1262.63	-1261.23	-1261.32	-1261.46	731.98	3.47
TPSSh	SVP	-1262.48	-1262.54	-1262.63	-1261.23	-1261.33	-1261.47	729.68	3.15
TPSSh	TZV	-1262.45	-1262.70	-1262.79	-1261.41	-1261.50	-1261.64	722.54	2.14
TPSSh	TZVP	-1262.65	-1262.70	-1262.79	-1261.41	-1261.50	-1261.64	722.65	2.14
TPSSh	QZVP	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.46	2.41
TPSSh	def2SV	-1262.48	-1262.73	-1262.63	-1261.23	-1261.33	-1261.47	729.68	3.15
TPSSh	def2SVP	-1262.48	-1262.54	-1262.63	-1261.23	-1261.33	-1261.47	730.47	3.26
TPSSh	def2SVPP	-1262.48	-1262.54	-1262.63	-1261.23	-1261.33	-1261.47	729.68	3.15
TPSSh	def2TZV	-1262.65	-1262.70	-1262.79	-1261.41	-1261.50	-1261.64	722.54	2.14
TPSSh	def2TZVP	-1262.65	-1262.70	-1262.79	-1261.41	-1261.50	-1261.64	723.31	2.25
TPSSh	def2TZVPP	-1262.65	-1262.70	-1262.79	-1261.41	-1261.50	-1261.64	723.84	2.32
TPSSh	def2QZV	-1262.67	-1262.73	-1262.82	-1261.43	-1261.53	-1261.67	723.00	2.20
TPSSh	def2QZVP	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.46	2.41
TPSSh	def2QZVPP	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.55	2.42
tHCTHhyb	3012 0/27 1 1	-1248.40	-1249.02	-1249.14	-1248.02	-1248.09	-1248.26	553.21	21.80
tHCTHhyb	6-31g	-1243.40	-1249.02	-1249.14	-1243.02	-1243.03	-1243.20	721.55	2.00
tHCTHhyb	6-31g(d,p)	-1262.49	-1262.54	-1262.64	-1261.25	-1261.34	-1261.48	721.81	2.03
tHCTHhyb	6-31+g	-1262.51	-1262.56	-1262.65	-1261.25	-1261.35	-1261.49	728.09	2.92
tHCTHhyb	6-31+g(d,p)	-1262.51	-1262.56	-1262.65	-1261.25	-1261.35	-1261.49	728.33	2.96
tHCTHhyb	6-31++g	-1262.51	-1262.56	-1262.65	-1261.25	-1261.35	-1261.49	728.09	2.92
tHCTHhyb	6-31++g 6-31++g(d,p)	-1262.51	-1262.56	-1262.65	-1261.25	-1261.35	-1261.49	728.33	2.96
tHCTHhyb	cc-pVDZ	-1262.67	-1262.72	-1262.82	-1261.42	-1261.51	-1261.66	728.34	2.96
tHCTHhyb	cc-pVTZ	-1262.67	-1262.69	-1262.82	-1261.42	-1261.51	-1261.66	726.75	2.73
tHCTHhyb	cc-pVIZ	-1262.68	-1262.73	-1262.82	-1261.43	-1261.52	-1261.67	727.63	2.86
tHCTHhyb	AUG-cc-pVDZ	-1262.67	-1262.68	-1262.82	-1261.42	-1261.52	-1261.66	728.26	2.95
tHCTHhyb	AUG-cc-pVTZ	-1262.67	-1262.73	-1262.82	-1261.42	-1261.52	-1261.66	726.76	2.73
tHCTHhyb	AUG-cc-pVQZ	-1262.68	-1262.73	-1262.82	-1261.43	-1261.52	-1261.67	727.63	2.86
511 C 1 1111y D	110 G-00-P V QZ	-1202.00	-1202.10	-1202.02	-1201.40	-1201.02	-1201.01	121.00	2.00

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

D 1	D	-		_			0	3IE	OAE
Functional	Basis set	1	3	5	2	4	6	Kcal/mol	%Error
tHCTHhyb	SV	-1262.48	-1262.53	-1262.63	-1261.21	-1261.31	-1261.46	734.12	3.77
tHCTHhyb	SVP	-1262.48	-1262.53	-1262.63	-1261.22	-1261.31	-1261.46	731.92	3.46
tHCTHhyb	TZV	-1262.64	-1262.70	-1262.79	-1261.39	-1261.49	-1261.64	725.24	2.52
tHCTHhyb	TZVP	-1262.65	-1262.70	-1262.79	-1261.39	-1261.49	-1261.64	725.42	2.54
tHCTHhyb	QZVP	-1262.67	-1262.73	-1262.82	-1261.42	-1261.52	-1261.66	727.06	2.78
tHCTHhyb	def2SV	-1262.48	-1262.53	-1262.63	-1261.22	-1261.31	-1261.46	731.92	3.46
tHCTHhyb	def2SVP	-1262.48	-1262.54	-1262.63	-1261.22	-1261.31	-1261.46	732.50	3.55
tHCTHhyb	def2SVPP	-1262.48	-1262.53	-1262.63	-1261.22	-1261.31	-1261.46	731.92	3.46
tHCTHhyb	def2TZV	-1262.64	-1262.70	-1262.79	-1261.39	-1261.49	-1261.64	725.24	2.52
tHCTHhyb	def2TZVP	-1262.65	-1262.70	-1262.79	-1261.39	-1261.49	-1261.64	725.91	2.61
tHCTHhyb	def2TZVPP	-1262.65	-1262.70	-1262.79	-1261.40	-1261.49	-1261.64	726.31	2.67
tHCTHhyb	def2QZV	-1262.67	-1262.73	-1262.82	-1261.42	-1261.52	-1261.66	725.97	2.62
tHCTHhyb	def2QZVP	-1262.67	-1262.73	-1262.82	-1261.42	-1261.52	-1261.66	727.06	2.78
tHCTHhyb	def2QZVPP	-1262.67	-1262.73	-1262.82	-1261.42	-1261.52	-1261.66	727.11	2.78
BMK		-1248.03	-1248.35	-1248.40	-1247.39	-1247.37	-1247.53	547.08	22.67
BMK	6-31g	-1261.96	-1262.01	-1262.09	-1260.74	-1260.83	-1260.95	713.64	0.88
BMK	6-31g(d,p)	-1261.96	-1262.01	-1262.09	-1260.74	-1260.83	-1260.95	714.01	0.93
BMK	6-31+g	-1261.97	-1262.02	-1262.11	-1260.74	-1260.83	-1260.96	720.83	1.90
BMK	6-31+g(d,p)	-1261.97	-1262.02	-1262.11	-1260.74	-1260.83	-1260.96	721.19	1.95
BMK	6-31++g	-1261.97	-1262.02	-1262.11	-1260.74	-1260.83	-1260.96	720.83	1.90
BMK	6-31++g(d,p)	-1261.97	-1262.02	-1262.11	-1260.74	-1260.83	-1260.96	721.19	1.95
BMK	cc-pVDZ	-1262.13	-1262.14	-1262.26	-1260.91	-1261.00	-1261.12	716.21	1.24
BMK	cc-pVTZ	-1262.13	-1262.18	-1262.27	-1260.91	-1261.00	-1261.13	715.45	1.13
BMK	cc-pVQZ	-1262.14	-1262.19	-1262.27	-1260.92	-1261.01	-1261.13	715.75	1.18
BMK	AUG-cc-pVDZ	-1262.13	-1262.14	-1262.26	-1260.91	-1261.00	-1261.12	716.08	1.22
BMK	AUG-cc-pVTZ	-1262.13	-1262.15	-1262.27	-1260.91	-1260.96	-1261.13	715.45	1.14
BMK	AUG-cc-pVQZ	-1262.14	-1262.19	-1262.27	-1260.92	-1261.01	-1261.13	715.73	1.18
BMK	SV	-1261.94	-1261.99	-1262.07	-1260.70	-1260.79	-1260.92	722.23	2.09
BMK	SVP	-1261.94	-1261.99	-1262.07	-1260.71	-1260.80	-1260.93	720.77	1.89
BMK	TZV	-1262.10	-1262.15	-1262.23	-1260.88	-1260.97	-1261.10	712.91	0.78
BMK	TZVP	-1262.10	-1262.15	-1262.24	-1260.88	-1260.97	-1261.10	713.10	0.80
BMK	QZVP	-1262.13	-1262.18	-1262.27	-1260.91	-1261.00	-1261.13	716.31	1.26
BMK	def2SV	-1261.94	-1261.99	-1262.07	-1260.71	-1260.80	-1260.93	720.77	1.89
BMK	def2SVP	-1261.94	-1261.99	-1262.07	-1260.71	-1260.80	-1260.93	721.43	1.98
BMK	def2SVPP	-1261.94	-1261.99	-1262.07	-1260.71	-1260.80	-1260.93	720.77	1.89
BMK	def2TZV	-1262.10	-1262.15	-1262.23	-1260.88	-1260.97	-1261.10	712.91	0.78
BMK	def2TZVP	-1262.10	-1262.15	-1262.24	-1260.88	-1260.97	-1261.10	713.48	0.86
BMK	def2TZVPP	-1262.10	-1262.15	-1262.24	-1260.89	-1260.94	-1261.10	713.40	0.92
BMK	def2QZV	-1262.13	-1262.18	-1262.27	-1260.91	-1261.00	-1261.13	715.10	1.09
BMK	def2QZVP	-1262.13	-1262.18	-1262.27	-1260.91	-1261.00	-1261.13	716.31	1.26
BMK	def2QZVPP	-1262.13	-1262.18	-1262.27	-1260.91	-1261.00	-1261.13	716.39	1.27
HISSbPBE	GOLD OF VII	-1248.65	-1248.86	-1248.97	-1247.85	-1247.92	-1248.09	551.99	21.97
HISSbPBE	6-31g	-1248.03	-1243.30	-1248.37	-1247.83	-1247.92	-1243.09	716.89	1.34
HISSbPBE	6-31g(d,p)	-1262.29	-1262.34	-1262.44	-1261.07	-1261.20	-1261.30	717.28	1.39
HISSbPBE	6-31+g	-1262.30	-1262.35	-1262.46	-1261.07	-1261.21	-1261.31	722.90	2.19
HISSbPBE	6-31+g(d,p)	-1262.30	-1262.35	-1262.46	-1261.07	-1261.21	-1261.31	723.57	2.19
HISSbPBE	6-31++g	-1262.30	-1262.35	-1262.46	-1261.07	-1261.21	-1261.31	722.90	2.19
HISSbPBE	6-31++g(d,p)	-1262.30	-1262.35	-1262.46	-1261.07	-1261.21	-1261.31	723.57	2.19
HISSbPBE	cc-pVDZ	-1262.46	-1262.51	-1262.40	-1261.07	-1261.37	-1261.47	724.83	2.46
HISSOPBE	cc-pVTZ	-1262.46	-1262.51	-1262.62	-1261.23	-1261.37	-1261.47	722.61	2.46
HISSIPBE	cc-pV1Z	-1262.47	-1262.52	-1262.63	-1261.24	-1261.29	-1261.47	723.50	2.13
THOODEDE	cc-bvQz	-1202.41	-1202.02	-1202.03	-1201.24	-1201.36	-1201.46	123.30	4.41

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

D .: 1	D : 4		9	_			C	3IE	07.15
Functional	Basis set	1	3	5	2	4	6	Kcal/mol	%Error
HISSbPBE	AUG-cc-pVDZ	-1262.46	-1262.52	-1262.62	-1261.23	-1261.29	-1261.47	724.23	2.38
HISSbPBE	AUG-cc-pVTZ	-1262.47	-1262.52	-1262.62	-1261.24	-1261.29	-1261.47	722.64	2.15
HISSbPBE	AUG-cc-pVQZ	-1262.47	-1262.52	-1262.63	-1261.24	-1261.29	-1261.48	723.50	2.27
HISSbPBE	SV	-1262.28	-1262.32	-1262.43	-1261.03	-1261.17	-1261.27	730.78	3.30
HISSbPBE	SVP	-1262.28	-1262.33	-1262.43	-1261.03	-1261.09	-1261.27	728.96	3.05
HISSbPBE	TZV	-1262.44	-1262.49	-1262.60	-1261.21	-1261.35	-1261.45	721.28	1.96
HISSbPBE	TZVP	-1262.44	-1262.49	-1262.60	-1261.21	-1261.26	-1261.45	721.53	1.99
HISSbPBE	QZVP	-1262.47	-1262.52	-1262.63	-1261.24	-1261.29	-1261.47	723.40	2.26
HISSbPBE	def2SV	-1262.28	-1262.33	-1262.43	-1261.03	-1261.17	-1261.27	728.44	2.97
HISSbPBE	def2SVP	-1262.28	-1262.33	-1262.43	-1261.03	-1261.09	-1261.27	729.17	3.07
HISSbPBE	def2SVPP	-1262.28	-1262.33	-1262.43	-1261.03	-1261.09	-1261.27	728.44	2.97
HISSbPBE	def2TZV	-1262.44	-1262.49	-1262.60	-1261.21	-1261.35	-1261.45	721.28	1.96
HISSbPBE	def2TZVP	-1262.44	-1262.49	-1262.60	-1261.21	-1261.35	-1261.45	721.99	2.06
HISSbPBE	def2TZVPP	-1262.44	-1262.49	-1262.60	-1261.21	-1261.27	-1261.45	722.51	2.13
HISSbPBE	def2QZV	-1262.47	-1262.52	-1262.62	-1261.24	-1261.38	-1261.47	722.12	2.08
HISSbPBE	def2QZVP	-1262.47	-1262.52	-1262.63	-1261.24	-1261.38	-1261.47	723.41	2.26
HISSbPBE	def2QZVPP	-1262.47	-1262.52	-1262.63	-1261.24	-1261.30	-1261.47	723.02	2.21
X3LYP	40126/2711	-1248.78	-1248.97	-1249.09	-1247.95	-1248.02	-1248.19	563.25	20.38
X3LYP	6-31g	-1262.42	-1262.47	-1262.57	-1261.19	-1261.28	-1261.42	719.32	1.68
X3LYP	6-31g(d,p)	-1262.42	-1262.47	-1262.57	-1261.19	-1261.28	-1261.42	719.64	1.73
X3LYP	6-31+g	-1262.44	-1262.49	-1262.58	-1261.19	-1261.29	-1261.43	726.67	2.72
X3LYP	6-31+g(d,p)	-1262.44	-1262.49	-1262.58	-1261.19	-1261.29	-1261.43	726.97	2.76
X3LYP	6-31++g	-1262.44	-1262.49	-1262.58	-1261.19	-1261.29	-1261.43	726.67	2.72
X3LYP	6-31++g 6-31++g(d,p)	-1262.44	-1262.49	-1262.58	-1261.19	-1261.29	-1261.43	726.97	2.76
X3LYP	cc-pVDZ	-1262.44	-1262.49	-1262.75	-1261.19	-1261.45	-1261.43	727.55	2.70
		-1262.60							
X3LYP X3LYP	cc-pVTZ cc-pVQZ		-1262.66	-1262.75	-1261.36	-1261.45	-1261.59	726.08 726.42	2.64
		-1262.61	-1262.66	-1262.75	-1261.36	-1261.46	-1261.60		2.69
X3LYP	AUG-cc-pVDZ	-1262.60	-1262.65	-1262.75	-1261.35	-1261.45	-1261.59	727.44	2.83
X3LYP	AUG-cc-pVTZ	-1262.60	-1262.66	-1262.75	-1261.36	-1261.45	-1261.59	726.10	2.64
X3LYP	AUG-cc-pVQZ	-1262.61	-1262.66	-1262.75	-1261.36	-1261.42	-1261.60	726.42	2.69
X3LYP	SV	-1262.41	-1262.46	-1262.56	-1261.15	-1261.24	-1261.39	734.40	3.81
X3LYP	SVP	-1262.41	-1262.46	-1262.56	-1261.15	-1261.25	-1261.39	732.42	3.53
X3LYP	TZV	-1262.58	-1262.63	-1262.72	-1261.33	-1261.43	-1261.57	724.30	2.39
X3LYP	TZVP	-1262.58	-1262.63	-1262.72	-1261.33	-1261.43	-1261.57	724.51	2.42
X3LYP	QZVP	-1262.61	-1262.62	-1262.75	-1261.36	-1261.45	-1261.59	726.44	2.69
X3LYP	def2SV	-1262.41	-1262.46	-1262.56	-1261.15	-1261.25	-1261.39	732.42	3.53
X3LYP	def2SVP	-1262.41	-1262.47	-1262.56	-1261.15	-1261.25	-1261.39	733.07	3.63
X3LYP	def2SVPP	-1262.41	-1262.46	-1262.56	-1261.15	-1261.25	-1261.39	732.42	3.53
X3LYP	def2TZV	-1262.58	-1262.63	-1262.72	-1261.33	-1261.43	-1261.57	724.30	2.39
X3LYP	def2TZVP	-1262.58	-1262.63	-1262.72	-1261.33	-1261.43	-1261.57	724.94	2.48
X3LYP	def2TZVPP	-1262.58	-1262.63	-1262.72	-1261.33	-1261.39	-1261.57	725.43	2.55
X3LYP	def2QZV	-1262.61	-1262.66	-1262.75	-1261.36	-1261.45	-1261.59	725.25	2.52
X3LYP	def2QZVP	-1262.61	-1262.62	-1262.75	-1261.36	-1261.45	-1261.59	726.44	2.69
X3LYP	def2QZVPP	-1262.61	-1262.66	-1262.75	-1261.36	-1261.45	-1261.59	726.53	2.70
BHandH		-1246.94	-1247.21	-1247.45	-1246.28	-1246.32	-1246.56	556.49	21.34
BHandH	6-31g	-1260.67	-1260.73	-1260.84	-1259.46	-1259.56	-1259.73	699.70	1.09
BHandH	6-31g(d,p)	-1260.67	-1260.73	-1260.84	-1259.46	-1259.56	-1259.73	700.11	1.03
BHandH	6-31+g	-1260.69	-1260.75	-1260.86	-1259.46	-1259.57	-1259.73	705.38	0.29
BHandH	6-31+g(d,p)	-1260.69	-1260.75	-1260.86	-1259.46	-1259.57	-1259.73	705.77	0.23
BHandH	6-31++g	-1260.69	-1260.75	-1260.86	-1259.46	-1259.57	-1259.73	705.38	0.29
BHandH	6-31++g(d,p)	-1260.69	-1260.75	-1260.86	-1259.46	-1259.57	-1259.73	705.77	0.23

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE	%Error
			_				_	Kcal/mol	
BHandH BHandH	cc-pVDZ cc-pVTZ	-1260.85 -1260.85	-1260.91 -1260.88	-1261.02 -1261.02	-1259.62 -1259.63	-1259.73 -1259.74	-1259.89 -1259.90	706.76 704.49	0.09
BHandH	cc-pV1Z cc-pVQZ	-1260.86	-1260.88	-1261.02	-1259.63	-1259.74	-1259.90	704.49	0.41
BHandH	AUG-cc-pVDZ	-1260.86	-1260.88	-1261.03	-1259.63	-1259.74	-1259.90	704.80	0.30
BHandH	AUG-cc-pVTZ	-1260.85	-1260.88	-1261.02	-1259.62	-1259.73	-1259.90	704.50	0.11
BHandH BHandH	AUG-cc-pVQZ SV	-1260.86 -1260.66	-1260.92 -1260.68	-1261.03 -1260.83	-1259.63 -1259.42	-1259.74 -1259.53	-1259.90 -1259.70	704.85 712.40	0.36 0.70
BHandH	SVP	-1260.66	-1260.08	-1260.83	-1259.42		-1259.70	712.40	0.70
BHandH	TZV	-1260.83	-1260.72	-1260.83	-1259.45	-1259.54 -1259.71	-1259.70	702.87	0.42
BHandH	TZVP	-1260.83	-1260.89	-1261.00	-1259.60	-1259.71	-1259.88	703.00	0.63
	QZVP	-1260.86	-1260.89	-1261.00	-1259.60	-1259.71	-1259.88	703.00	0.03
BHandH	def2SV	-1260.66	-1260.92	-1261.03	-1259.03	-1259.74	-1259.90	710.37	0.37
BHandH									
BHandH	def2SVP	-1260.66	-1260.73	-1260.83	-1259.43	-1259.54	-1259.70	711.16	0.53
BHandH	def2SVPP	-1260.66	-1260.72	-1260.83	-1259.43	-1259.54	-1259.70	710.37	0.42
BHandH	def2TZV	-1260.83	-1260.89	-1260.99	-1259.60	-1259.71	-1259.87	702.87	0.64
BHandH	def2TZVP	-1260.83	-1260.89	-1261.00	-1259.60	-1259.71	-1259.88	703.54	0.55
BHandH	def2TZVPP	-1260.83	-1260.89	-1261.00	-1259.60	-1259.71	-1259.88	703.98	0.49
BHandH	def2QZV	-1260.85	-1260.91	-1261.02	-1259.63	-1259.69	-1259.90	703.41	0.57
BHandH	def2QZVP	-1260.86	-1260.92	-1261.03	-1259.63	-1259.70	-1259.90	704.78	0.37
BHandH	def2QZVPP	-1260.86	-1260.88	-1261.03	-1259.63	-1259.74	-1259.90	704.86	0.36
BHandHLYP	0.01	-1248.75	-1249.02	-1249.24	-1248.10	-1248.17	-1248.35	559.84	20.86
BHandHLYP	6-31g	-1262.47	-1262.52	-1262.62	-1261.25	-1261.34	-1261.50	705.92	0.21
BHandHLYP	6-31g(d,p)	-1262.47	-1262.52	-1262.62	-1261.25	-1261.35	-1261.50	706.40	0.14
BHandHLYP	6-31+g	-1262.48	-1262.54	-1262.64	-1261.25	-1261.35	-1261.50	711.31	0.55
BHandHLYP	6-31+g(d,p)	-1262.48	-1262.54	-1262.64	-1261.25	-1261.35	-1261.50	711.78	0.62
BHandHLYP	6-31++g	-1262.48	-1262.54	-1262.64	-1261.25	-1261.35	-1261.50	711.31	0.55
BHandHLYP	6-31++g(d,p)	-1262.48	-1262.54	-1262.64	-1261.25	-1261.35	-1261.50	711.78	0.62
BHandHLYP	cc-pVDZ	-1262.65	-1262.66	-1262.80	-1261.41	-1261.51	-1261.66	713.29	0.83
BHandHLYP	cc-pVTZ	-1262.65	-1262.70	-1262.80	-1261.42	-1261.52	-1261.67	710.70	0.46
BHandHLYP	cc-pVQZ	-1262.65	-1262.70	-1262.80	-1261.42	-1261.52	-1261.67	711.05	0.51
BHandHLYP	AUG-cc-pVDZ	-1262.65	-1262.66	-1262.80	-1261.41	-1261.51	-1261.66	713.14	0.81
BHandHLYP	AUG-cc-pVTZ	-1262.65	-1262.66	-1262.80	-1261.42	-1261.52	-1261.67	710.71	0.47
BHandHLYP	AUG-cc-pVQZ	-1262.65	-1262.67	-1262.80	-1261.42	-1261.48	-1261.67	711.05	0.51
BHandHLYP	SV	-1262.46	-1262.51	-1262.61	-1261.21	-1261.31	-1261.46	719.25	1.67
BHandHLYP	SVP	-1262.46	-1262.51	-1262.61	-1261.21	-1261.31	-1261.47	717.02	1.36
BHandHLYP	TZV	-1262.62	-1262.67	-1262.77	-1261.39	-1261.49	-1261.64	708.92	0.21
BHandHLYP	TZVP	-1262.62	-1262.67	-1262.77	-1261.39	-1261.49	-1261.64	709.05	0.23
BHandHLYP	QZVP	-1262.65	-1262.70	-1262.80	-1261.42	-1261.52	-1261.67	711.07	0.52
BHandHLYP	def2SV	-1262.46	-1262.51	-1262.61	-1261.21	-1261.31	-1261.47	717.02	1.36
BHandHLYP	def2SVP	-1262.46	-1262.51	-1262.61	-1261.22	-1261.32	-1261.47	717.95	1.49
BHandHLYP	def2SVPP	-1262.46	-1262.51	-1262.61	-1261.21	-1261.31	-1261.47	717.02	1.36
BHandHLYP	def2TZV	-1262.62	-1262.67	-1262.77	-1261.39	-1261.49	-1261.64	708.92	0.21
BHandHLYP	def2TZVP	-1262.62	-1262.67	-1262.77	-1261.39	-1261.49	-1261.64	709.75	0.33
BHandHLYP	def2TZVPP	-1262.62	-1262.68	-1262.78	-1261.40	-1261.49	-1261.64	710.27	0.40
BHandHLYP	def2QZV	-1262.65	-1262.70	-1262.80	-1261.42	-1261.52	-1261.67	709.47	0.29
BHandHLYP	def2QZVP	-1262.65	-1262.70	-1262.80	-1261.42	-1261.52	-1261.67	711.07	0.52
BHandHLYP	def2QZVPP	-1262.65	-1262.70	-1262.80	-1261.42	-1261.48	-1261.67	711.15	0.53
M06HF	0.04	-1248.72	-1248.96	-1249.14	-1248.00	-1248.12	-1248.21	587.16	17.00
M06HF	6-31g	-1262.48	-1262.55	-1262.64	-1261.27	-1261.38	-1261.49	722.11	2.08
M06HF	6-31g(d,p)	-1262.48	-1262.55	-1262.64	-1261.27	-1261.38	-1261.49	722.45	2.12
M06HF	6-31+g	-1262.49	-1262.56	-1262.65	-1261.28	-1261.39	-1261.49	728.53	2.98

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
M06HF	6-31+g(d,p)	-1262.49	-1262.56	-1262.65	-1261.28	-1261.39	-1261.49	728.86	3.03
M06HF	6-31++g	-1262.49	-1262.56	-1262.65	-1261.28	-1261.39	-1261.49	728.53	2.98
M06HF	6-31++g(d,p)	-1262.49	-1262.56	-1262.65	-1261.28	-1261.39	-1261.49	728.86	3.03
M06HF	cc-pVDZ	-1262.68	-1262.71	-1262.83	-1261.46	-1261.51	-1261.67	728.84	3.03
M06HF	cc-pVTZ	-1262.68	-1262.71	-1262.84	-1261.46	-1261.57	-1261.68	728.22	2.94
M06HF	cc-pVQZ	-1262.69	-1262.76	-1262.85	-1261.47	-1261.53	-1261.69	730.16	3.21
M06HF	AUG-cc-pVDZ	-1262.68	-1262.71	-1262.83	-1261.46	-1261.52	-1261.67	728.82	3.03
M06HF	AUG-cc-pVTZ	-1262.68	-1262.75	-1262.84	-1261.46	-1261.57	-1261.68	728.28	2.95
M06HF	AUG-cc-pVQZ	-1262.69	-1262.76	-1262.85	-1261.47	-1261.53	-1261.69	730.24	3.23
M06HF	SV	-1262.49	-1262.56	-1262.65	-1261.25	-1261.37	-1261.48	734.46	3.82
M06HF	SVP	-1262.49	-1262.56	-1262.65	-1261.26	-1261.37	-1261.48	733.84	3.73
M06HF	TZV	-1262.65	-1262.72	-1262.80	-1261.43	-1261.54	-1261.65	727.15	2.79
M06HF	TZVP	-1262.65	-1262.72	-1262.81	-1261.43	-1261.54	-1261.65	727.59	2.85
M06HF	QZVP	-1262.69	-1262.76	-1262.85	-1261.47	-1261.58	-1261.69	728.87	3.03
M06HF	def2SV	-1262.49	-1262.56	-1262.65	-1261.26	-1261.37	-1261.48	733.84	3.73
M06HF	def2SVP	-1262.49	-1262.56	-1262.65	-1261.26	-1261.37	-1261.48	734.45	3.82
M06HF	def2SVPP	-1262.49	-1262.56	-1262.65	-1261.26	-1261.37	-1261.48	733.84	3.73
M06HF	def2TZV	-1262.65	-1262.72	-1262.80	-1261.43	-1261.54	-1261.65	727.15	2.79
M06HF	def2TZVP	-1262.65	-1262.72	-1262.81	-1261.43	-1261.54	-1261.65	727.96	2.90
M06HF	def2TZVPP	-1262.65	-1262.72	-1262.81	-1261.44	-1261.54	-1261.65	728.59	2.99
M06HF	def2QZV	-1262.69	-1262.76	-1262.85	-1261.47	-1261.54	-1261.69	727.64	2.86
M06HF	def2QZVP	-1262.69	-1262.76	-1262.85	-1261.47	-1261.58	-1261.69	728.87	3.03
M06HF	def2QZVPP	-1262.69	-1262.76	-1262.85	-1261.47	-1261.58	-1261.69	728.95	3.04
M06L	deizQZVII	-1248.38	-1249.02	-1249.18	-1248.09	-1248.17	-1248.33	533.45	24.59
M06L	6-31g	-1262.45	-1262.49	-1262.58	-1240.03	-1261.30	-1261.46	706.55	0.12
M06L	6-31g(d,p)	-1262.45	-1262.49	-1262.59	-1261.21	-1261.30	-1261.46	706.90	0.12
M06L	6-31+g	-1262.47	-1262.49	-1262.60	-1261.21	-1261.30	-1261.46	711.96	0.64
M06L	6-31+g(d,p)	-1262.47	-1262.51	-1262.60	-1261.22	-1261.30	-1261.46	712.29	0.69
M06L	6-31++g	-1262.47	-1262.51	-1262.60	-1261.21	-1261.30	-1261.46	711.96	0.64
M06L	6-31++g(d,p)	-1262.47	-1262.51	-1262.60	-1261.22	-1261.30	-1261.46	712.29	0.69
M06L	cc-pVDZ	-1262.62	-1262.68	-1262.76	-1261.38	-1261.50	-1261.63	707.66	0.03
M06L	cc-pVTZ	-1262.62	-1262.66	-1262.76	-1261.38	-1261.47	-1261.64	703.78	0.51
M06L	cc-pV1Z	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	705.26	0.31
M06L	AUG-cc-pVDZ	-1262.62	-1262.68	-1262.76	-1261.38	-1261.47	-1261.63	707.50	0.31
M06L	AUG-cc-pVTZ	-1262.62	-1262.66	-1262.76	-1261.38	-1261.47	-1261.64	703.82	0.51
M06L	AUG-cc-pVQZ	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	705.26	0.31
M06L	SV	-1262.43	-1262.49	-1262.76	-1261.17	-1261.26	-1261.43	712.23	0.68
M06L	SVP	-1262.43	-1262.47	-1262.56	-1261.17	-1261.27	-1261.44	708.64	0.03
M06L	TZV	-1262.43	-1262.47	-1262.73	-1261.17	-1261.27	-1261.44	702.43	0.17
M06L	TZVP	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.43	0.71
M06L	QZVP	-1262.69	-1262.64	-1262.76	-1261.38	-1261.45	-1261.61	702.28	0.75
M06L	def2SV	-1262.62	-1262.47	-1262.76	-1261.38	-1261.47	-1261.64	704.95	0.33
	def2SVP	-1262.43							0.17
M06L M06L	def2SVPP	-1262.43	-1262.47 -1262.47	-1262.57 -1262.56	-1261.18 -1261.17	-1261.31 -1261.30	-1261.44 -1261.44	709.26 708.64	0.26
M06L	def2TZV	-1262.43	-1262.47	-1262.73	-1261.17	-1261.30	-1261.44	708.04	0.17
M06L	def2TZVP	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.43	0.71
M06L	def2TZVPP	-1262.59	-1262.66	-1262.73	-1261.36	-1261.45	-1261.61	702.86	0.63
M06L	def2QZV	-1262.69	-1262.66	-1262.76	-1261.38	-1261.49	-1261.61	702.90	0.51
M06L	def2QZVP	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	703.80	0.35
M06L	def2QZVPP	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	704.95	0.34
SOGGA11	ueizQZVFF	-1262.62	-1262.69	-1262.76	-1201.38	-1201.47	-1201.04	440.87	37.68
SOGGAII		-1240.10	-1240.70	-1240.03	-1241.91	-1240.02	-1240.13	440.01	31.00

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
SOGGA11	6-31g	-1262.33	-1262.58	-1262.64	-1261.26	-1261.38	-1261.47	733.90	3.74
SOGGA11	6-31g(d,p)	-1262.46	-1262.58	-1262.63	-1261.35	-1261.38	-1261.47	733.13	3.63
SOGGA11	6-31+g	-1262.41	-1262.60	-1262.65	-1261.27	-1261.39	-1261.47	740.91	4.73
SOGGA11	6-31+g(d,p)	-1262.47	-1262.59	-1262.65	-1261.35	-1261.39	-1261.47	741.05	4.75
SOGGA11	6-31++g	-1262.41	-1262.60	-1262.65	-1261.35	-1261.39	-1261.47	740.91	4.73
SOGGA11	6-31++g(d,p)	-1262.46	-1262.59	-1262.65	-1261.35	-1261.39	-1261.47	741.05	4.75
SOGGA11	cc-pVDZ	-1262.50	-1262.76	-1262.82	-1261.50	-1261.54	-1261.63	742.14	4.91
SOGGA11	cc-pVTZ	-1262.69	-1262.76	-1262.82	-1261.51	-1261.55	-1261.64	742.07	4.90
SOGGA11	cc-pVQZ	-1262.52	-1262.76	-1262.82	-1261.52	-1261.56	-1261.65	738.01	4.32
SOGGA11	AUG-cc-pVDZ	-1262.53	-1262.75	-1262.82	-1261.50	-1261.46	-1261.63	742.16	4.91
SOGGA11	AUG-cc-pVTZ	-1262.69	-1262.76	-1262.81	-1261.51	-1261.55	-1261.64	737.50	4.25
SOGGA11	AUG-cc-pVQZ	-1262.69	-1262.77	-1262.82	-1261.52	-1261.56	-1261.65	737.80	4.29
SOGGA11	SV	-1262.48	-1262.58	-1262.64	-1261.30	-1261.34	-1261.44	750.64	6.11
SOGGA11	SVP	-1262.46	-1262.57	-1262.64	-1261.30	-1261.35	-1261.45	748.35	5.79
SOGGA11	TZV	-1262.54	-1262.73	-1262.80	-1261.48	-1261.52	-1261.61	747.04	5.60
SOGGA11	TZVP	-1262.66	-1262.74	-1262.80	-1261.48	-1261.52	-1261.61	747.29	5.64
SOGGA11	QZVP	-1262.69	-1262.77	-1262.82	-1261.51	-1261.56	-1261.64	739.70	4.56
SOGGA11	def2SV	-1262.46	-1262.58	-1262.64	-1261.30	-1261.35	-1261.45	746.90	5.58
SOGGA11	def2SVP	-1262.47	-1262.58	-1262.64	-1261.30	-1261.35	-1261.45	748.41	5.79
SOGGA11	def2SVPP	-1262.46	-1262.58	-1262.64	-1261.30	-1261.35	-1261.45	746.90	5.58
SOGGA11	def2TZV	-1262.63	-1262.61	-1262.80	-1261.48	-1261.52	-1261.61	747.37	5.65
SOGGA11	def2TZVP	-1262.66	-1262.74	-1262.80	-1261.48	-1261.52	-1261.61	746.99	5.59
SOGGA11	def2TZVPP	-1262.66	-1262.74	-1262.80	-1261.48	-1261.52	-1261.61	747.15	5.62
SOGGA11	def2QZV	-1262.65	-1262.63	-1262.82	-1261.51	-1261.55	-1261.64	739.36	4.52
SOGGA11	def2QZVP	-1262.69	-1262.77	-1262.82	-1261.51	-1261.56	-1261.64	739.70	4.56
SOGGA11	def2QZVPP	-1262.69	-1262.77	-1262.82	-1261.51	-1261.56	-1261.64	740.18	4.63
M11L	dci2@ZVII	-1248.33	-1248.43	-1248.94	-1248.07	-1248.04	-1248.21	459.78	35.01
M11L	6-31g	-1262.66	-1262.65	-1262.68	-1261.41	-1261.43	-1261.52	731.65	3.42
M11L	6-31g(d,p)	-1262.67	-1262.66	-1262.69	-1261.41	-1261.43	-1261.52	732.63	3.56
M11L	6-31+g	-1262.68	-1262.67	-1262.70	-1261.41	-1261.44	-1261.53	734.53	3.83
M11L	6-31+g(d,p)	-1262.68	-1262.67	-1262.70	-1261.42	-1261.44	-1261.53	735.47	3.97
M11L	6-31++g	-1262.68	-1262.67	-1262.70	-1261.41	-1261.44	-1261.53	734.53	3.83
M11L	6-31++g(d,p)	-1262.68	-1262.67	-1262.70	-1261.42	-1261.44	-1261.53	735.47	3.97
M11L	cc-pVDZ	-1262.84	-1262.82	-1262.85	-1261.57	-1261.58	-1261.67	744.46	5.24
M11L	cc-pVTZ	-1262.85	-1262.84	-1262.87	-1261.59	-1261.61	-1261.69	736.24	4.07
M11L	cc-pVQZ	-1262.86	-1262.85	-1262.88	-1261.60	-1261.62	-1261.71	735.19	3.93
M11L	AUG-cc-pVDZ	-1262.84	-1262.83	-1262.85	-1261.57	-1261.58	-1261.67	744.03	5.17
M11L	AUG-cc-pVTZ	-1262.85	-1262.84	-1262.87	-1261.59	-1261.61	-1261.69	736.31	4.08
M11L	AUG-cc-pVQZ	-1262.86	-1262.85	-1262.88	-1261.60	-1261.62	-1261.71	735.28	3.94
M11L	SV SV	-1262.63	-1262.62	-1262.65	-1261.35	-1261.37	-1261.45	752.62	6.39
M11L	SVP	-1262.64	-1262.62	-1262.66	-1261.36	-1261.38	-1261.46	746.91	5.58
M11L	TZV	-1262.81	-1262.79	-1262.83	-1261.55	-1261.57	-1261.66	735.19	3.93
M11L	TZVP	-1262.81	-1262.80	-1262.83	-1261.55	-1261.57	-1261.66	734.87	3.88
M11L	QZVP	-1262.88	-1262.87	-1262.90	-1261.62	-1261.67	-1261.73	735.41	3.96
M11L	def2SV	-1262.64	-1262.62	-1262.66	-1261.36	-1261.38	-1261.46	746.91	5.58
M11L	def2SVP	-1262.65	-1262.63	-1262.66	-1261.37	-1261.38	-1261.46	748.74	5.84
M11L	def2SVPP	-1262.64	-1262.62	-1262.66	-1261.36	-1261.38	-1261.46	746.91	5.58
M11L	def2TZV	-1262.81	-1262.79	-1262.83	-1261.55	-1261.57	-1261.66	735.19	3.93
M11L	def2TZVP	-1262.82	-1262.80	-1262.83	-1261.56	-1261.57	-1261.66	736.86	4.16
M11L	def2TZVPP	-1262.82	-1262.81	-1262.83	-1261.56	-1261.61	-1261.66	737.46	4.10
M11L	def2QZV	-1262.82	-1262.86	-1262.89	-1261.61	-1261.63	-1261.73	732.53	3.55
1V1.1.1.L	UCIZWZ V	-1202.01	-1202.00	-1202.09	-1201.01	-1201.03	-1201.73	102.00	5.55

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
M11L	def2QZVP	-1262.88	-1262.87	-1262.90	-1261.62	-1261.67	-1261.73	735.41	3.96
M11L	def2QZVPP	-1262.88	-1262.87	-1262.90	-1261.62	-1261.64	-1261.73	735.49	3.97
MN12L		-1247.45	-1247.37	-1247.86	-1246.94	-1246.95	-1247.03	520.95	26.36
MN12L	6-31g	-1262.21	-1262.24	-1262.29	-1260.99	-1261.06	-1261.14	721.08	1.93
MN12L	6-31g(d,p)	-1262.22	-1262.24	-1262.29	-1260.99	-1261.06	-1261.14	722.13	2.08
MN12L	6-31+g	-1262.24	-1262.26	-1262.31	-1261.00	-1261.06	-1261.15	732.05	3.48
MN12L	6-31+g(d,p)	-1262.24	-1262.27	-1262.32	-1261.00	-1261.07	-1261.15	733.06	3.62
MN12L	6-31++g	-1262.24	-1262.26	-1262.31	-1261.00	-1261.06	-1261.15	732.05	3.48
MN12L	6-31++g(d,p)	-1262.24	-1262.27	-1262.32	-1261.00	-1261.07	-1261.15	733.06	3.62
MN12L	cc-pVDZ	-1262.39	-1262.42	-1262.48	-1261.16	-1261.23	-1261.32	729.42	3.11
MN12L	cc-pVTZ	-1262.41	-1262.44	-1262.50	-1261.18	-1261.25	-1261.33	731.96	3.47
MN12L	cc-pVQZ	-1262.43	-1262.46	-1262.52	-1261.20	-1261.27	-1261.35	734.17	3.78
MN12L	AUG-cc-pVDZ	-1262.40	-1262.42	-1262.48	-1261.16	-1261.25	-1261.32	729.57	3.13
MN12L	AUG-cc-pVTZ	-1262.41	-1262.44	-1262.50	-1261.18	-1261.27	-1261.33	731.98	3.47
MN12L	AUG-cc-pVQZ	-1262.43	-1262.46	-1262.52	-1261.20	-1261.27	-1261.35	734.18	3.78
MN12L	SV	-1262.16	-1262.19	-1262.25	-1260.92	-1260.99	-1261.08	729.91	3.18
MN12L	SVP	-1262.17	-1262.19	-1262.25	-1260.93	-1261.00	-1261.09	728.39	2.96
MN12L	TZV	-1262.37	-1262.40	-1262.46	-1261.14	-1261.21	-1261.30	728.91	3.04
MN12L	TZVP	-1262.38	-1262.40	-1262.46	-1261.15	-1261.21	-1261.30	728.87	3.03
MN12L	QZVP	-1262.43	-1262.46	-1262.52	-1261.20	-1261.27	-1261.35	732.45	3.54
MN12L	def2SV	-1262.17	-1262.19	-1262.25	-1260.93	-1261.00	-1261.09	728.39	2.96
MN12L	def2SVP	-1262.17	-1262.20	-1262.25	-1260.94	-1261.01	-1261.09	730.69	3.29
MN12L	def2SVPP	-1262.17	-1262.19	-1262.25	-1260.93	-1261.00	-1261.09	728.39	2.96
MN12L	def2TZV	-1262.37	-1262.40	-1262.46	-1261.14	-1261.21	-1261.30	728.91	3.04
MN12L	def2TZVP	-1262.38	-1262.41	-1262.46	-1261.15	-1261.22	-1261.30	731.14	3.35
MN12L	def2TZVPP	-1262.38	-1262.41	-1262.47	-1261.16	-1261.22	-1261.30	732.18	3.50
MN12L	def2QZV	-1262.43	-1262.45	-1262.51	-1261.22	-1261.26	-1261.35	728.91	3.04
MN12L	def2QZVP	-1262.43	-1262.46	-1262.52	-1261.20	-1261.27	-1261.35	732.45	3.54
MN12L	def2QZVPP	-1262.43	-1262.46	-1262.52	-1261.20	-1261.27	-1261.35	732.53	3.55
N12		-1248.40	-1249.05	-1249.13	-1248.11	-1248.14	-1248.24	559.61	20.89
N12	6-31g	-1262.85	-1262.93	-1262.99	-1261.68	-1261.68	-1261.81	737.83	4.30
N12	6-31g(d,p)	-1262.85	-1262.90	-1262.99	-1261.68	-1261.68	-1261.81	738.06	4.33
N12	6-31+g	-1262.87	-1262.92	-1263.00	-1261.69	-1261.72	-1261.82	744.87	5.29
N12	6-31+g(d,p)	-1262.87	-1262.92	-1263.00	-1261.69	-1261.72	-1261.82	745.09	5.33
N12	6-31++g	-1262.87	-1262.92	-1263.00	-1261.69	-1261.72	-1261.82	744.87	5.29
N12	6-31++g(d,p)	-1262.87	-1262.92	-1263.00	-1261.69	-1261.72	-1261.82	745.09	5.33
N12	cc-pVDZ	-1263.05	-1263.12	-1263.18	-1261.87	-1261.90	-1261.99	747.23	5.63
N12	cc-pVTZ	-1263.06	-1263.13	-1263.19	-1261.88	-1261.91	-1262.00	746.90	5.58
N12	cc-pVQZ	-1263.07	-1263.15	-1263.20	-1261.89	-1261.92	-1262.01	748.35	5.79
N12	AUG-cc-pVDZ	-1263.05	-1263.12	-1263.18	-1261.87	-1261.90	-1261.99	747.25	5.63
N12	AUG-cc-pVTZ	-1263.06	-1263.11	-1263.19	-1261.88	-1261.91	-1262.00	746.94	5.59
N12	AUG-cc-pVQZ	-1263.07	-1263.14	-1263.20	-1261.89	-1261.88	-1262.01	748.42	5.80
N12	SV	-1262.85	-1262.93	-1262.98	-1261.64	-1261.64	-1261.77	763.85	7.98
N12	SVP	-1262.85	-1262.93	-1262.99	-1261.65	-1261.68	-1261.77	760.28	7.47
N12	TZV	-1263.03	-1263.10	-1263.16	-1261.84	-1261.84	-1261.97	745.42	5.37
N12	TZVP	-1263.03	-1263.10	-1263.16	-1261.84	-1261.84	-1261.97	745.61	5.40
N12	QZVP	-1263.07	-1263.15	-1263.20	-1261.89	-1261.88	-1262.01	747.05	5.60
N12	def2SV	-1262.85	-1262.93	-1262.99	-1261.65	-1261.60	-1261.77	760.28	7.47
N12	def2SVP	-1262.85	-1262.93	-1262.99	-1261.65	-1261.60	-1261.77	760.79	7.54
	def2SVPP	-1262.85	-1262.90	-1262.99	-1261.65	-1261.60	-1261.77	760.28	7.47
N12	del 25 vii	1202.00	1202.00	1202.00	1201.00		1201	1.00.20	

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
N12	def2TZVP	-1263.03	-1263.10	-1263.16	-1261.84	-1261.84	-1261.97	745.99	5.45
N12	def2TZVPP	-1263.03	-1263.10	-1263.16	-1261.85	-1261.84	-1261.97	746.49	5.52
N12	def2QZV	-1263.07	-1263.14	-1263.20	-1261.89	-1261.88	-1262.01	745.97	5.45
N12	def2QZVP	-1263.07	-1263.15	-1263.20	-1261.89	-1261.88	-1262.01	747.05	5.60
N12	def2QZVPP	-1263.07	-1263.15	-1263.21	-1261.89	-1261.93	-1262.01	747.12	5.61
MN15L		-1247.04	-1247.33	-1247.57	-1246.41	-1246.48	-1246.72	532.24	24.76
MN15L	6-31g	-1262.40	-1262.46	-1262.58	-1261.18	-1261.30	-1261.51	673.14	4.85
MN15L	6-31g(d,p)	-1262.40	-1262.46	-1262.58	-1261.18	-1261.30	-1261.51	673.61	4.78
MN15L	6-31+g	-1262.42	-1262.48	-1262.60	-1261.19	-1261.31	-1261.51	681.31	3.69
MN15L	6-31+g(d,p)	-1262.42	-1262.48	-1262.60	-1261.19	-1261.31	-1261.51	681.76	3.63
MN15L	6-31++g	-1262.42	-1262.48	-1262.60	-1261.19	-1261.31	-1261.51	681.31	3.69
MN15L	6-31++g(d,p)	-1262.42	-1262.48	-1262.60	-1261.19	-1261.31	-1261.51	681.76	3.63
MN15L	cc-pVDZ	-1262.58	-1262.65	-1262.76	-1261.35	-1261.47	-1261.68	681.71	3.63
MN15L	cc-pVTZ	-1262.58	-1262.65	-1262.77	-1261.36	-1261.48	-1261.68	680.24	3.84
MN15L	cc-pVQZ	-1262.59	-1262.66	-1262.77	-1261.37	-1261.48	-1261.69	680.68	3.78
MN15L	AUG-cc-pVDZ	-1262.58	-1262.65	-1262.76	-1261.35	-1261.47	-1261.68	681.70	3.64
MN15L	AUG-cc-pVTZ	-1262.58	-1262.65	-1262.77	-1261.36	-1261.48	-1261.68	680.31	3.83
MN15L	AUG-cc-pVQZ	-1262.59	-1262.65	-1262.77	-1261.37	-1261.48	-1261.69	680.74	3.77
MN15L	SV	-1262.38	-1262.44	-1262.56	-1261.14	-1261.26	-1261.47	685.28	3.13
MN15L	SVP	-1262.38	-1262.44	-1262.56	-1261.14	-1261.26	-1261.47	682.81	3.48
MN15L	TZV	-1262.55	-1262.62	-1262.74	-1261.33	-1261.45	-1261.65	679.42	3.96
MN15L	TZVP	-1262.55	-1262.62	-1262.74	-1261.33	-1261.45	-1261.66	679.37	3.97
MN15L	QZVP	-1262.61	-1262.67	-1262.79	-1261.38	-1261.50	-1261.71	680.09	3.86
MN15L	def2SV	-1262.38	-1262.44	-1262.56	-1261.14	-1261.26	-1261.47	682.81	3.48
MN15L	def2SVP	-1262.38	-1262.44	-1262.56	-1261.15	-1261.27	-1261.47	683.29	3.41
MN15L	def2SVPP	-1262.38	-1262.44	-1262.56	-1261.14	-1261.26	-1261.47	682.81	3.48
MN15L	def2TZV	-1262.55	-1262.62	-1262.74	-1261.33	-1261.45	-1261.65	679.42	3.96
MN15L	def2TZVP	-1262.56	-1262.62	-1262.74	-1261.33	-1261.45	-1261.66	679.93	3.89
MN15L	def2TZVPP	-1262.56	-1262.62	-1262.74	-1261.33	-1261.46	-1261.66	680.26	3.84
MN15L	def2QZV	-1262.61	-1262.67	-1262.79	-1261.38	-1261.50	-1261.71	678.94	4.03
MN15L	def2QZVP	-1262.61	-1262.67	-1262.79	-1261.38	-1261.50	-1261.71	680.09	3.86
MN15L	def2QZVPP	-1262.61	-1262.68	-1262.79	-1261.38	-1261.52	-1261.71	680.22	3.84
VSXC		-1249.01	-1249.32	-1249.62	-1248.52	-1248.49	-1248.75	546.95	22.68
VSXC	6-31g	-1262.93	-1263.00	-1263.11	-1261.79	-1261.85	-1261.99	704.74	0.38
VSXC	6-31g(d,p)	-1262.93	-1263.00	-1263.11	-1261.79	-1261.85	-1261.99	704.98	0.35
VSXC	6-31+g	-1262.95	-1263.01	-1263.13	-1261.80	-1261.86	-1261.99	711.19	0.53
VSXC	6-31+g(d,p)	-1262.95	-1263.02	-1263.13	-1261.80	-1261.86	-1261.99	711.42	0.56
VSXC	6-31++g	-1262.95	-1263.01	-1263.13	-1261.80	-1261.86	-1261.99	711.19	0.53
VSXC	6-31++g(d,p)	-1262.95	-1263.02	-1263.13	-1261.80	-1261.86	-1261.99	711.42	0.56
VSXC	cc-pVDZ	-1263.11	-1263.20	-1263.29	-1261.96	-1262.02	-1262.15	713.66	0.88
VSXC	cc-pVTZ	-1263.12	-1263.18	-1263.29	-1261.96	-1262.03	-1262.16	711.65	0.60
VSXC	cc-pVQZ	-1263.12	-1263.21	-1263.30	-1261.97	-1261.99	-1262.16	712.11	0.66
VSXC	AUG-cc-pVDZ	-1263.11	-1263.21	-1263.29	-1261.96	-1261.93	-1262.15	713.59	0.87
VSXC	AUG-cc-pVTZ	-1263.12	-1263.20	-1263.29	-1261.96	-1262.03	-1262.16	711.68	0.60
VSXC	AUG-cc-pVQZ	-1263.12	-1263.21	-1263.30	-1261.97	-1261.99	-1262.16	712.13	0.67
VSXC	SV	-1262.92	-1263.01	-1263.10	-1261.71	-1261.72	-1261.95	720.74	1.88
TIGHTO	CVD	-1262.92	-1263.01	-1263.10	-1261.71	-1261.78	-1261.95	718.41	1.55
VSXC	SVP	1202.02							
VSXC	TZV	-1263.09	-1263.18	-1263.26	-1261.93	-1261.96	-1262.13	710.28	0.40
					-1261.93 -1261.93	-1261.96 -1261.96	-1262.13 -1262.13	710.48	0.40 0.43
VSXC	TZV	-1263.09	-1263.18	-1263.26					

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
VSXC	def2SVP	-1262.92	-1262.99	-1263.10	-1261.76	-1261.82	-1261.95	718.93	1.63
VSXC	def2SVPP	-1262.92	-1262.98	-1263.10	-1261.75	-1261.73	-1261.95	718.41	1.55
VSXC	def2TZV	-1263.09	-1263.18	-1263.26	-1261.93	-1261.96	-1262.13	710.28	0.40
VSXC	def2TZVP	-1263.09	-1263.15	-1263.26	-1261.94	-1261.96	-1262.13	710.99	0.50
VSXC	def2TZVPP	-1263.09	-1263.18	-1263.27	-1261.94	-1261.96	-1262.13	711.44	0.57
VSXC	def2QZV	-1263.12	-1263.18	-1263.29	-1261.96	-1261.99	-1262.16	710.80	0.48
VSXC	def2QZVP	-1263.12	-1263.21	-1263.30	-1261.97	-1261.99	-1262.16	711.86	0.63
VSXC	def2QZVPP	-1263.12	-1263.21	-1263.30	-1261.97	-1261.92	-1262.16	711.92	0.64
tHCTH	-	-1248.74	-1249.62	-1249.62	-1248.68	-1248.75	-1248.90	453.48	35.90
tHCTH	6-31g	-1262.89	-1263.16	-1263.25	-1261.90	-1261.90	-1262.09	726.19	2.65
tHCTH	6-31g(d,p)	-1262.92	-1263.16	-1263.25	-1261.90	-1261.97	-1262.09	726.22	2.66
tHCTH	6-31+g	-1262.91	-1263.18	-1263.26	-1261.91	-1261.97	-1262.10	730.56	3.27
tHCTH	6-31+g(d,p)	-1263.10	-1263.18	-1263.26	-1261.91	-1261.97	-1262.10	730.93	3.32
tHCTH	6-31++g	-1263.10	-1263.18	-1263.26	-1261.91	-1261.97	-1262.10	730.56	3.27
tHCTH	6-31++g(d,p)	-1263.10	-1263.18	-1263.26	-1261.91	-1261.97	-1262.10	730.93	3.32
tHCTH	cc-pVDZ	-1263.26	-1263.35	-1263.43	-1262.08	-1262.14	-1262.27	732.20	3.50
tHCTH	cc-pVTZ	-1263.27	-1263.35	-1263.44	-1262.08	-1262.15	-1262.27	730.09	3.20
tHCTH	cc-pVQZ	-1263.27	-1263.36	-1263.43	-1262.09	-1262.15	-1262.28	725.65	2.58
tHCTH	AUG-cc-pVDZ	-1263.26	-1263.36	-1263.43	-1262.08	-1262.05	-1262.27	730.87	3.31
tHCTH	AUG-cc-pVTZ	-1263.27	-1263.35	-1263.44	-1262.08	-1262.15	-1262.27	730.25	3.23
tHCTH	AUG-cc-pV IZ	-1263.27	-1263.36	-1263.44	-1262.09	-1262.15	-1262.28	731.67	3.43
tHCTH	SV SV	-1263.07	-1263.16	-1263.24	-1261.87	-1261.93	-1262.26	739.37	4.52
tHCTH	SVP	-1263.08	-1263.16	-1263.24	-1261.87	-1261.94	-1262.07	735.52	3.97
tHCTH	TZV	-1263.24	-1263.32	-1263.41	-1262.05	-1262.12	-1262.25	729.25	3.09
tHCTH	TZVP	-1263.24	-1263.32	-1263.41	-1262.05	-1262.12	-1262.25	728.65	3.00
tHCTH	QZVP	-1263.27	-1263.35	-1263.44	-1262.09	-1262.12	-1262.28	730.08	3.20
tHCTH	def2SV	-1263.27	-1263.16	-1263.25	-1261.87	-1261.87	-1262.28	736.37	4.09
tHCTH	def2SVP	-1263.08	-1263.16	-1263.25	-1261.88	-1261.86	-1262.07	736.69	4.14
tHCTH	def2SVPP	-1263.08	-1263.16	-1263.24	-1261.87	-1261.86	-1262.07	735.74	4.14
tHCTH	def2TZV	-1263.08	-1263.32		-1262.05	-1262.12	-1262.07	728.92	3.04
tHCTH	def2TZVP	-1263.24	-1263.32	-1263.41 -1263.40	-1262.06	-1262.12	-1262.25	725.23	2.52
	def2TZVPP	-1263.24							3.18
tHCTH tHCTH			-1263.33	-1263.41	-1262.06	-1262.12	-1262.25	729.94 729.44	
	def2QZV	-1263.27	-1263.35	-1263.44	-1262.08	-1262.15	-1262.28		3.11
tHCTH tHCTH	def2QZVP def2QZVPP	-1263.27	-1263.36	-1263.44	-1262.09	-1262.15 -1262.15	-1262.28	730.08	3.20 3.26
	deizQZVFF	-1263.27	-1263.35	-1263.44	-1262.09		-1262.28	730.50	22.35
B97D	C 21	-1248.83	-1249.44	-1249.59	-1248.50	-1248.57	-1248.71	549.31	
B97D	6-31g	-1262.91	-1263.00	-1263.07 -1263.07	-1261.75	-1261.73	-1261.92 -1261.92	720.79	1.89
B97D	6-31g(d,p)	-1262.91	-1262.99		-1261.75	-1261.73		721.00	1.92
B97D	6-31+g	-1262.93	-1262.90	-1263.09	-1261.75	-1261.74	-1261.93	726.67	2.72
B97D	6-31+g(d,p)	-1262.93	-1263.01	-1263.09	-1261.76	-1261.73	-1261.93	726.60	2.71
B97D	6-31++g	-1262.93	-1262.90	-1263.09	-1261.75	-1261.73	-1261.93	728.43	2.97
B97D	6-31++g(d,p)	-1262.93	-1263.01	-1263.09	-1261.76	-1261.73	-1261.93	726.60	2.71
B97D	cc-pVDZ	-1263.10	-1263.18	-1263.26	-1261.92	-1261.90	-1262.10	728.05	2.92
B97D	cc-pVTZ	-1263.10	-1263.18	-1263.26	-1261.93	-1261.90	-1262.10	726.74	2.73
B97D	cc-pVQZ	-1263.10	-1263.19	-1263.27	-1261.93	-1261.90	-1262.11	727.83	2.88
B97D	AUG-cc-pVDZ	-1263.10	-1263.18	-1263.26	-1261.92	-1261.98	-1262.10	728.01	2.91
B97D	AUG-cc-pVTZ	-1263.10	-1263.18	-1263.26	-1261.93	-1261.98	-1262.10	726.76	2.73
B97D	AUG-cc-pVQZ	-1263.10	-1263.19	-1263.27	-1261.93	-1261.99	-1262.11	727.83	2.89
B97D	SV	-1262.90	-1262.98	-1263.06	-1261.71	-1261.77	-1261.89	734.91	3.89
						1001 50			
B97D B97D	SVP TZV	-1262.90 -1263.07	-1262.98 -1263.15	-1263.06 -1263.23	-1261.72 -1261.90	-1261.78 -1261.96	-1261.90 -1262.08	731.10 723.45	3.35 2.27

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
B97D	TZVP	-1263.07	-1263.15	-1263.23	-1261.90	-1261.96	-1262.08	724.96	2.48
B97D	QZVP	-1263.10	-1263.18	-1263.26	-1261.93	-1261.99	-1262.10	727.14	2.79
B97D	def2SV	-1262.90	-1262.99	-1263.06	-1261.72	-1261.70	-1261.90	731.18	3.36
B97D	def2SVP	-1262.90	-1262.98	-1263.07	-1261.72	-1261.78	-1261.90	732.45	3.54
B97D	def2SVPP	-1262.90	-1262.98	-1263.06	-1261.72	-1261.70	-1261.90	731.18	3.36
B97D	def2TZV	-1263.07	-1263.15	-1263.23	-1261.90	-1261.96	-1262.08	723.50	2.27
B97D	def2TZVP	-1263.07	-1263.14	-1263.23	-1261.90	-1261.96	-1262.08	725.22	2.52
B97D	def2TZVPP	-1263.07	-1263.09	-1263.23	-1261.90	-1261.96	-1262.08	726.24	2.66
B97D	def2QZV	-1263.10	-1263.09	-1263.26	-1261.93	-1261.98	-1262.10	725.82	2.60
B97D	def2QZVP	-1263.10	-1263.18	-1263.26	-1261.93	-1261.99	-1262.10	727.14	2.79
B97D	def2QZVPP	-1263.10	-1263.10	-1263.26	-1261.93	-1261.99	-1262.10	727.18	2.79
HCTH		-1249.18	-1249.52	-1249.50	-1248.56	-1248.63	-1248.79	463.44	34.49
HCTH	6-31g	-1262.80	-1263.05	-1263.14	-1261.71	-1261.85	-1261.98	726.56	2.71
HCTH	6-31g(d,p)	-1262.85	-1263.05	-1263.14	-1261.70	-1261.85	-1261.98	726.60	2.71
HCTH	6-31+g	-1262.80	-1263.06	-1263.15	-1261.79	-1261.86	-1261.98	730.59	3.27
НСТН	6-31+g(d,p)	-1262.82	-1263.07	-1263.15	-1261.79	-1261.80	-1261.98	731.62	3.42
HCTH	6-31++g	-1262.98	-1263.06	-1263.15	-1261.79	-1261.80	-1261.98	730.59	3.27
HCTH	6-31++g(d,p)	-1262.98	-1263.06	-1263.15	-1261.79	-1261.86	-1261.98	732.13	3.49
HCTH	cc-pVDZ	-1263.05	-1263.23	-1263.31	-1261.95	-1262.02	-1262.15	729.58	3.13
HCTH	cc-pVTZ	-1263.14	-1263.23	-1263.32	-1261.96	-1262.03	-1262.16	729.80	3.16
HCTH	cc-pVQZ	-1263.03	-1263.24	-1263.32	-1261.97	-1262.03	-1262.16	730.44	3.25
HCTH	AUG-cc-pVDZ	-1262.98	-1263.23	-1263.32	-1261.95	-1261.96	-1262.15	732.26	3.51
HCTH	AUG-cc-pVTZ	-1263.01	-1263.23	-1263.32	-1261.96	-1262.03	-1262.16	729.55	3.13
HCTH	AUG-cc-pVQZ	-1263.05	-1263.24	-1263.32	-1261.97	-1262.03	-1262.16	729.13	3.07
HCTH	SV	-1262.79	-1263.04	-1263.12	-1261.74	-1261.75	-1261.94	740.50	4.68
НСТН	SVP	-1262.86	-1262.98	-1263.13	-1261.75	-1261.82	-1261.95	737.97	4.32
HCTH	TZV	-1262.94	-1263.15	-1263.29	-1261.93	-1262.00	-1262.13	728.82	3.02
HCTH	TZVP	-1262.95	-1263.20	-1263.29	-1261.93	-1262.00	-1262.13	728.86	3.03
HCTH	QZVP	-1263.01	-1263.18	-1263.32	-1261.96	-1262.03	-1262.16	730.11	3.21
HCTH	def2SV	-1262.78	-1263.04	-1263.12	-1261.75	-1261.74	-1261.95	736.85	4.16
HCTH	def2SVP	-1262.81	-1263.04	-1263.13	-1261.75	-1261.82	-1261.95	738.17	4.35
HCTH	def2SVPP	-1262.83	-1262.93	-1263.13	-1261.75	-1261.74	-1261.95	737.87	4.30
HCTH	def2TZV	-1262.94	-1263.20	-1263.29	-1261.93	-1261.92	-1262.13	728.19	2.94
HCTH	def2TZVP	-1262.94	-1263.15	-1263.29	-1261.94	-1262.00	-1262.13	729.17	3.07
HCTH	def2TZVPP	-1263.07	-1263.15	-1263.29	-1261.94	-1262.00	-1262.13	729.23	3.08
HCTH	def2QZV	-1263.10	-1263.17	-1263.32	-1261.88	-1262.03	-1262.16	730.01	3.19
HCTH	def2QZVP	-1263.10	-1263.17	-1263.32	-1261.96	-1262.03	-1262.16	730.01	3.19
HCTH	def2QZVPP	-1263.01	-1263.24	-1263.32	-1261.96	-1261.94	-1262.16	730.03	3.20
HCTH93	GCIZ WZZ VII	-1248.80	-1249.62	-1249.59	-1248.66	-1248.63	-1248.88	464.31	34.37
HCTH93	6-31g	-1248.80	-1249.02	-1249.39	-1248.00	-1248.03	-1248.88	720.23	1.81
HCTH93	6-31g(d,p)	-1262.89	-1263.12	-1263.21	-1261.87	-1261.94	-1262.07	720.23	1.83
HCTH93	6-31+g	-1263.06	-1263.14	-1263.23	-1261.88	-1261.87	-1262.07	725.24	2.52
HCTH93	6-31+g(d,p)	-1263.06	-1263.14	-1263.23	-1261.88	-1261.87	-1262.07	726.83	2.74
HCTH93	6-31++g	-1263.06	-1263.14	-1263.23	-1261.88	-1261.85	-1262.07	725.24	2.74
HCTH93	6-31++g(d,p)	-1263.06	-1263.14	-1263.23	-1261.88	-1261.94	-1262.07	726.83	2.74
HCTH93	cc-pVDZ	-1263.22	-1263.30	-1263.39	-1262.04	-1262.02	-1262.23	727.22	2.80
HCTH93	cc-pVTZ	-1263.22	-1263.32	-1263.40	-1262.04	-1262.02	-1262.24	725.34	2.53
HCTH93	cc-pV1Z	-1263.23	-1263.31	-1263.40	-1262.05	-1262.11	-1262.24	726.11	2.64
HCTH93	AUG-cc-pVDZ	-1263.22	-1263.31	-1263.39	-1262.04	-1262.12	-1262.24	720.11	2.79
HCTH93	AUG-cc-pVTZ	-1263.22	-1263.31	-1263.40	-1262.04	-1262.02	-1262.24	725.36	2.79
HCTH93	AUG-cc-pVQZ	-1263.22	-1263.31	-1263.40	-1262.05	-1262.12	-1262.24	726.11	2.64
110 11130	nog-cc-pvQZ	-1400.40	-1200.02	-1200.40	-1202.00	-1404.14	-1404.44	140.11	4.04

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
HCTH93	SV	-1263.03	-1263.11	-1263.20	-1261.83	-1261.81	-1262.03	734.44	3.82
HCTH93	SVP	-1263.03	-1263.12	-1263.20	-1261.84	-1261.82	-1262.03	731.40	3.39
HCTH93	TZV	-1263.19	-1263.17	-1263.37	-1262.02	-1262.08	-1262.21	721.97	2.06
HCTH93	TZVP	-1263.20	-1263.29	-1263.37	-1262.02	-1262.08	-1262.21	723.75	2.31
HCTH93	QZVP	-1263.22	-1263.31	-1263.40	-1261.98	-1262.03	-1262.24	725.79	2.60
HCTH93	def2SV	-1263.03	-1263.01	-1263.20	-1261.84	-1261.82	-1262.03	731.38	3.39
HCTH93	def2SVP	-1263.03	-1263.01	-1263.20	-1261.84	-1261.90	-1262.03	733.36	3.67
HCTH93	def2SVPP	-1263.03	-1263.01	-1263.20	-1261.84	-1261.82	-1262.03	731.38	3.39
HCTH93	def2TZV	-1263.19	-1263.22	-1263.37	-1262.02	-1262.08	-1262.21	721.98	2.06
HCTH93	def2TZVP	-1263.20	-1263.28	-1263.37	-1262.02	-1262.09	-1262.22	724.47	2.41
HCTH93	def2TZVPP	-1263.20	-1263.22	-1263.37	-1262.02	-1262.09	-1262.22	724.87	2.47
HCTH93	def2QZV	-1263.22	-1263.25	-1263.40	-1262.05	-1262.11	-1262.24	724.60	2.43
HCTH93	def2QZVP	-1263.22	-1263.31	-1263.40	-1262.05	-1262.11	-1262.24	725.79	2.60
HCTH93	def2QZVPP	-1263.22	-1263.25	-1263.40	-1261.97	-1262.11	-1262.24	725.84	2.60
HCTH147	dei2@2711	-1249.05	-1249.52	-1249.67	-1248.55	-1248.53	-1248.78	556.99	21.26
HCTH147	6-31g	-1262.77	-1262.92	-1263.12	-1261.77	-1261.84	-1261.97	722.41	2.12
HCTH147	6-31g(d,p)	-1262.80	-1262.92	-1263.12	-1261.77	-1261.84	-1261.97	721.22	1.95
HCTH147	6-31+g	-1262.84	-1263.04	-1263.13	-1261.78	-1261.84	-1261.97	728.82	3.03
HCTH147	6-31+g(d,p)	-1262.81	-1262.94	-1263.13	-1261.78	-1261.84	-1261.97	727.04	2.77
HCTH147	6-31++g	-1262.91	-1263.04	-1263.13	-1261.78	-1261.76	-1261.97	728.82	3.03
HCTH147	6-31++g(d,p)	-1262.81	-1263.04	-1263.13	-1261.78	-1261.76	-1261.97	727.04	2.77
HCTH147	cc-pVDZ	-1263.07	-1263.21	-1263.30	-1261.78	-1261.92	-1262.13	729.65	3.14
HCTH147	cc-pVTZ	-1263.08	-1263.21	-1263.30	-1261.88	-1262.01	-1262.14	728.31	2.95
HCTH147	cc-pV1Z	-1262.97	-1263.15	-1263.31	-1261.88	-1262.01	-1262.14	728.97	3.05
HCTH147	AUG-cc-pVDZ	-1262.96	-1263.13	-1263.30	-1261.93	-1261.94	-1262.14	729.61	3.14
HCTH147	AUG-cc-pVTZ	-1263.13	-1263.22	-1263.30	-1261.94	-1262.01	-1262.14	729.01	2.95
HCTH147	AUG-cc-pV1Z	-1262.98	-1263.21	-1263.31	-1261.95	-1262.01	-1262.14	728.97	3.05
HCTH147	SV	-1262.75	-1263.22	-1263.11	-1261.73	-1262.02	-1262.14	738.18	4.35
	SVP								
HCTH147	TZV	-1262.75	-1262.96 -1263.08	-1263.10	-1261.74	-1261.80	-1261.94	733.77	3.73
HCTH147	TZVP	-1262.95		-1263.27	-1261.83	-1261.98	-1262.11	726.48	2.69
HCTH147 HCTH147	QZVP	-1262.92	-1263.18	-1263.27	-1261.83	-1261.98	-1262.11	726.71 728.52	2.73 2.98
		-1263.13	-1263.21	-1263.30	-1261.95	-1262.01	-1262.14		
HCTH147	def2SV	-1262.93	-1263.02	-1263.11	-1261.74	-1261.73	-1261.94	734.90	3.89
HCTH147 HCTH147	def2SVP def2SVPP	-1262.93	-1263.03 -1263.02	-1263.10	-1261.74	-1261.80	-1261.94 -1261.94	733.77 734.90	3.72 3.89
HCTH147	def2TZV	-1262.93		-1263.11	-1261.74	-1261.80 -1261.98		734.90	
		-1262.95	-1263.18	-1263.27	-1261.92		-1262.11		2.70
HCTH147 HCTH147	def2TZVP def2TZVPP	-1262.94 -1262.92	-1263.19 -1263.12	-1263.27 -1263.28	-1261.92 -1261.92	-1261.98	-1262.12 -1262.12	727.12 727.89	2.78 2.89
		-1262.92				-1261.99			
HCTH147 HCTH147	def2QZV def2QZVP		-1263.15 -1263.10	-1263.30 -1263.30	-1261.95 -1261.95	-1262.01 -1262.01	-1262.14 -1262.14	727.41 728.52	2.83 2.98
HCTH147	def2QZVP def2QZVPP	-1263.08 -1263.13	-1263.10	-1263.30	-1261.95	-1262.01	-1262.14	728.52	3.01
HCTH407	ueizQZVFF	-1203.13	-1203.22	-1263.30	-1261.95	-1201.93	-1262.14	558.47	21.06
	6-31g								
HCTH407		-1262.79	-1263.05	-1263.14	-1261.71	-1261.85	-1261.98 -1261.98	726.57 726.60	2.71
HCTH407 HCTH407	6-31g(d,p) 6-31+g	-1262.85 -1262.83	-1263.05 -1263.06	-1263.14 -1263.15	-1261.70 -1261.79	-1261.85 -1261.86	-1261.98	730.59	2.71 3.27
HCTH407	6-31+g 6-31+g(d,p)								
	6-31+g(d,p) 6-31++g	-1262.98	-1263.07	-1263.15	-1261.79 -1261.79	-1261.80	-1261.98	732.70	3.57
HCTH407 HCTH407	6-31++g 6-31++g(d,p)	-1262.83 -1262.83	-1263.06 -1263.07	-1263.15 -1263.15	-1261.79	-1261.86 -1261.80	-1261.98 -1261.98	732.36 730.83	3.52
HCTH407	cc-pVDZ					-1261.80			3.31
HCTH407 HCTH407	cc-pVDZ cc-pVTZ	-1263.05	-1263.23 -1263.11	-1263.32 -1263.32	-1261.95	-1262.02	-1262.15 -1262.16	732.17 729.80	3.50
		-1263.14			-1261.96				3.16
HCTH407	cc-pVQZ	-1263.03	-1263.24	-1263.32	-1261.97	-1262.03	-1262.16	730.44	3.25

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
HCTH407	AUG-cc-pVDZ	-1262.98	-1263.23	-1263.32	-1261.95	-1261.95	-1262.15	732.26	3.51
HCTH407	AUG-cc-pVTZ	-1263.01	-1263.23	-1263.32	-1261.96	-1262.03	-1262.16	729.55	3.13
HCTH407	AUG-cc-pVQZ	-1262.99	-1263.18	-1263.32	-1261.97	-1262.03	-1262.16	730.37	3.24
HCTH407	SV	-1262.79	-1263.04	-1263.12	-1261.74	-1261.81	-1261.94	740.50	4.68
HCTH407	SVP	-1262.95	-1262.95	-1263.12	-1261.75	-1261.82	-1261.95	736.87	4.16
HCTH407	TZV	-1262.99	-1263.15	-1263.29	-1261.93	-1262.00	-1262.13	728.82	3.02
HCTH407	TZVP	-1263.01	-1263.20	-1263.29	-1261.93	-1262.00	-1262.13	728.83	3.03
HCTH407	QZVP	-1263.01	-1263.18	-1263.32	-1261.96	-1262.03	-1262.16	730.11	3.21
HCTH407	def2SV	-1262.83	-1263.16	-1263.13	-1261.75	-1261.74	-1261.95	737.31	4.23
HCTH407	def2SVP	-1262.83	-1263.04	-1263.13	-1261.75	-1261.74	-1261.95	738.17	4.25
HCTH407	def2SVPP	-1262.83	-1263.04	-1263.13	-1261.75	-1261.74	-1261.95	737.85	4.30
HCTH407	def2TZV	-1263.07	-1263.15	-1263.29	-1261.73	-1262.00	-1262.13	728.19	2.94
HCTH407	def2TZVP	-1262.94	-1263.15	-1263.29	-1261.94	-1262.00	-1262.13	729.13	3.07
HCTH407	def2TZVPP	-1263.05	-1263.13	-1263.29	-1261.94	-1262.00	-1262.13	729.13	3.08
HCTH407	def2QZV	-1263.10	-1263.13	-1263.32	-1261.88	-1262.03	-1262.16	730.02	3.19
HCTH407	def2QZVP	-1263.10	-1263.11	-1263.32	-1261.86	-1262.03	-1262.16	730.02	3.19
HCTH407	def2QZVPP	-1263.00	-1263.11	-1263.32	-1261.96	-1262.03	-1262.16	730.09	3.20
B2PLYP	deizQZVFF	-1203.00	-1203.18	-1203.32	-1201.90	-1202.03	-1202.10	555.88	21.42
B2PLYP	6-31g	-1248.45	-1248.73	-1248.97	-1247.81	-1247.84	-1248.08	695.90	1.63
B2PLYP	6-31g(d,p)	-1262.16	-1262.22	-1262.32	-1260.95	-1261.06	-1261.21	696.43	1.55
B2PLYP	6-31+g	-1262.18	-1262.22	-1262.32	-1260.95	-1261.06	-1261.21	701.25	0.87
					-1260.96		-1261.22	701.25	0.80
B2PLYP	6-31+g(d,p)	-1262.18	-1262.23	-1262.34 -1262.34		-1261.06			
B2PLYP	6-31++g	-1262.18	-1262.23		-1260.96	-1261.06	-1261.22	701.25	0.87
B2PLYP	6-31++g(d,p)	-1262.18	-1262.23	-1262.34	-1260.96	-1261.06 -1261.22	-1261.22	701.77	0.80
B2PLYP	cc-pVDZ	-1262.34	-1262.36	-1262.50	-1261.12		-1261.38	703.31	0.58
B2PLYP	cc-pVTZ	-1262.34	-1262.40	-1262.50	-1261.13	-1261.23	-1261.38	700.66	0.96
B2PLYP	cc-pVQZ	-1262.34	-1262.40	-1262.50	-1261.13	-1261.23	-1261.39	701.03	0.90
B2PLYP	AUG-cc-pVDZ	-1262.34	-1262.36	-1262.50	-1261.12	-1261.22	-1261.38	703.16	0.60
B2PLYP	AUG-cc-pVTZ	-1262.34	-1262.36	-1262.50	-1261.13	-1261.23 -1261.23	-1261.38	700.68	0.95
B2PLYP	AUG-cc-pVQZ SV	-1262.34	-1262.36	-1262.50	-1261.13		-1261.39	701.02	0.90
B2PLYP	SVP	-1262.15	-1262.20	-1262.31	-1260.92	-1261.02	-1261.18	708.99	0.22
B2PLYP		-1262.15	-1262.21	-1262.31	-1260.92	-1261.02	-1261.18	706.73	0.10
B2PLYP	TZV	-1262.31	-1262.37	-1262.47	-1261.10	-1261.20	-1261.36	698.82	1.22
B2PLYP	TZVP	-1262.31	-1262.37	-1262.47	-1261.10	-1261.20	-1261.36	698.93	1.20
B2PLYP	QZVP	-1262.34	-1262.40	-1262.50	-1261.13	-1261.23	-1261.39	701.02	0.91
B2PLYP	def2SV	-1262.15	-1262.21	-1262.31	-1260.92	-1261.02	-1261.18	706.73	0.10
B2PLYP	def2SVP	-1262.15	-1262.21	-1262.31	-1260.92	-1260.99	-1261.18	707.74	0.04
B2PLYP	def2SVPP	-1262.15	-1262.21	-1262.31	-1260.92	-1261.02	-1261.18	706.73	0.10
B2PLYP	def2TZV	-1262.31	-1262.37	-1262.47	-1261.10	-1261.20	-1261.36	698.82	1.22
B2PLYP	def2TZVP	-1262.31	-1262.37	-1262.47	-1261.10	-1261.20	-1261.36	699.71	1.09
B2PLYP	def2TZVPP	-1262.31	-1262.37	-1262.48	-1261.10	-1261.20	-1261.36	700.26	1.01
B2PLYP	def2QZV	-1262.34	-1262.39	-1262.50	-1261.12	-1261.23	-1261.39	699.32	1.15
B2PLYP	def2QZVP	-1262.34	-1262.40	-1262.50	-1261.13	-1261.23	-1261.39	701.02	0.91
B2PLYP	def2QZVPP	-1262.34	-1262.36	-1262.50	-1261.13	-1261.23	-1261.39	701.11	0.89
mPW2PLYP	0.01	-1248.48	-1248.76	-1249.00	-1247.83	-1247.88	-1248.11	557.02	21.26
mPW2PLYP	6-31g	-1262.19	-1262.24	-1262.35	-1260.98	-1261.08	-1261.24	696.13	1.60
mPW2PLYP	6-31g(d,p)	-1262.19	-1262.24	-1262.35	-1260.98	-1261.08	-1261.24	696.67	1.52
mPW2PLYP	6-31+g	-1262.20	-1262.26	-1262.36	-1260.98	-1261.09	-1261.24	701.56	0.83
mPW2PLYP	6-31+g(d,p)	-1262.20	-1262.26	-1262.36	-1260.99	-1261.09	-1261.24	702.08	0.75
mPW2PLYP	6-31++g	-1262.20	-1262.26	-1262.36	-1260.98	-1261.09	-1261.24	701.56	0.83
mPW2PLYP	6-31++g(d,p)	-1262.20	-1262.26	-1262.36	-1260.99	-1261.09	-1261.24	702.08	0.75

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE	%Error
							_	Kcal/mol	
mPW2PLYP	cc-pVDZ	-1262.37	-1262.38	-1262.53	-1261.15	-1261.21	-1261.41	703.77	0.52
mPW2PLYP	cc-pVTZ	-1262.37	-1262.39	-1262.53	-1261.15	-1261.22	-1261.41	701.06	0.90
mPW2PLYP	cc-pVQZ	-1262.37	-1262.43	-1262.53	-1261.16	-1261.26	-1261.41	701.45	0.84
mPW2PLYP	AUG-cc-pVDZ	-1262.37	-1262.42	-1262.53	-1261.15	-1261.25	-1261.41	703.62	0.54
mPW2PLYP	AUG-cc-pVTZ	-1262.37	-1262.42	-1262.53	-1261.15	-1261.25	-1261.41	701.09	0.90
mPW2PLYP	AUG-cc-pVQZ	-1262.37	-1262.39	-1262.53	-1261.16	-1261.26	-1261.41	701.45	0.84
mPW2PLYP	SV	-1262.18	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	709.25	0.26
mPW2PLYP	SVP	-1262.18	-1262.23	-1262.34	-1260.95	-1261.05	-1261.21	707.03	0.05
mPW2PLYP	TZV	-1262.34	-1262.39	-1262.50	-1261.12	-1261.23	-1261.39	699.20	1.16
mPW2PLYP	TZVP	-1262.34	-1262.39	-1262.50	-1261.12	-1261.23	-1261.39	699.31	1.15
mPW2PLYP	QZVP	-1262.37	-1262.42	-1262.53	-1261.15	-1261.25	-1261.41	701.45	0.84
mPW2PLYP	def2SV	-1262.18	-1262.23	-1262.34	-1260.95	-1261.05	-1261.21	707.03	0.05
mPW2PLYP	def2SVP	-1262.18	-1262.24	-1262.34	-1260.95	-1261.05	-1261.21	708.06	0.09
mPW2PLYP	def2SVPP	-1262.18	-1262.23	-1262.34	-1260.95	-1261.05	-1261.21	707.03	0.05
mPW2PLYP	def2TZV	-1262.34	-1262.39	-1262.50	-1261.12	-1261.23	-1261.39	699.20	1.16
mPW2PLYP	def2TZVP	-1262.34	-1262.40	-1262.50	-1261.13	-1261.23	-1261.39	700.13	1.03
mPW2PLYP	def2TZVPP	-1262.34	-1262.40	-1262.50	-1261.13	-1261.19	-1261.39	700.68	0.95
mPW2PLYP	def2QZV	-1262.37	-1262.42	-1262.53	-1261.15	-1261.25	-1261.41	699.73	1.09
mPW2PLYP	def2QZVP	-1262.37	-1262.42	-1262.53	-1261.15	-1261.25	-1261.41	701.45	0.84
mPW2PLYP	def2QZVPP	-1262.37	-1262.39	-1262.53	-1261.15	-1261.25	-1261.41	701.54	0.83
DSDPBEP86		-1248.13	-1248.43	-1248.68	-1247.27	-1247.60	-1247.81	548.48	22.47
DSDPBEP86	6-31g	-1261.78	-1261.84	-1261.96	-1260.59	-1260.70	-1260.87	682.03	3.59
DSDPBEP86	6-31g(d,p)	-1261.78	-1261.84	-1261.96	-1260.59	-1260.70	-1260.87	682.75	3.49
DSDPBEP86	6-31+g	-1261.79	-1261.85	-1261.97	-1260.59	-1260.70	-1260.88	686.16	3.01
DSDPBEP86	6-31+g(d,p)	-1261.80	-1261.86	-1261.97	-1260.60	-1260.70	-1260.88	686.86	2.91
DSDPBEP86	6-31++g	-1261.79	-1261.85	-1261.97	-1260.59	-1260.70	-1260.88	686.16	3.01
DSDPBEP86	6-31++g(d,p)	-1261.80	-1261.86	-1261.97	-1260.60	-1260.70	-1260.88	686.86	2.91
DSDPBEP86	cc-pVDZ	-1261.96	-1261.98	-1262.13	-1260.76	-1260.82	-1261.03	688.84	2.63
DSDPBEP86	cc-pVTZ	-1261.96	-1262.02	-1262.13	-1260.76	-1260.83	-1261.04	685.54	3.09
DSDPBEP86	cc-pVQZ	-1261.96	-1261.99	-1262.14	-1260.77	-1260.87	-1261.04	685.94	3.04
DSDPBEP86	AUG-cc-pVDZ	-1261.96	-1261.98	-1262.13	-1260.76	-1260.86	-1261.04	688.66	2.65
DSDPBEP86	AUG-cc-pVTZ	-1261.96	-1262.02	-1262.13	-1260.76	-1260.83	-1261.04	685.57	3.09
DSDPBEP86	AUG-cc-pVQZ	-1261.96	-1262.02	-1262.14	-1260.77	-1260.87	-1261.04	685.94	3.04
DSDPBEP86	SV	-1261.77	-1261.83	-1261.94	-1260.55	-1260.66	-1260.84	693.48	1.97
DSDPBEP86	SVP	-1261.77	-1261.83	-1261.95	-1260.56	-1260.67	-1260.84	690.99	2.32
DSDPBEP86	TZV	-1261.93	-1261.99	-1262.11	-1260.73	-1260.84	-1261.02	683.60	3.37
DSDPBEP86	TZVP	-1261.93	-1261.99	-1262.11	-1260.73	-1260.84	-1261.02	683.63	3.36
DSDPBEP86	QZVP	-1261.96	-1261.98	-1262.14	-1260.76	-1260.87	-1261.04	685.84	3.05
DSDPBEP86	def2SV	-1261.77	-1261.83	-1261.95	-1260.56	-1260.67	-1260.84	690.99	2.32
DSDPBEP86	def2SVP	-1261.77	-1261.83	-1261.95	-1260.56	-1260.67	-1260.84	692.26	2.14
DSDPBEP86	def2SVPP	-1261.77	-1261.83	-1261.95	-1260.56	-1260.67	-1260.84	690.99	2.32
DSDPBEP86	def2TZV	-1261.93	-1261.99	-1262.11	-1260.73	-1260.84	-1261.02	683.60	3.37
DSDPBEP86	def2TZVP	-1261.93	-1261.99	-1262.11	-1260.74	-1260.85	-1261.02	684.70	3.21
DSDPBEP86	def2TZVPP	-1261.93	-1261.99	-1262.11	-1260.74	-1260.81	-1261.02	685.27	3.13
DSDPBEP86	def2QZV	-1261.96	-1262.02	-1262.13	-1260.76	-1260.87	-1261.04	683.76	3.34
DSDPBEP86	def2QZVP	-1261.96	-1262.02	-1262.14	-1260.76	-1260.83	-1261.04	685.84	3.05
DSDPBEP86	def2QZVPP	-1261.96	-1261.98	-1262.14	-1260.76	-1260.87	-1261.04	685.94	3.04
PBE0DH		-1248.48	-1248.75	-1248.99	-1247.84	-1247.91	-1248.11	552.08	21.96
PBE0DH	6-31g	-1262.15	-1262.21	-1262.32	-1260.94	-1261.04	-1261.21	700.88	0.92
PBE0DH	6-31g(d,p)	-1262.15	-1262.21	-1262.33	-1260.94	-1261.04	-1261.21	701.42	0.85
PBE0DH	6-31+g	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	705.49	0.27
	1 ' 0	1							

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE	%Error
PBE0DH	6.21 + c(d p)	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	Kcal/mol 706.01	0.20
PBE0DH	6-31+g(d,p) 6-31++g	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	705.49	0.20
PBE0DH	6-31++g 6-31++g(d,p)	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	706.01	0.27
PBE0DH	cc-pVDZ	-1262.17	-1262.25	-1262.54	-1260.94	-1261.05	-1261.21	707.87	0.20
PBE0DH	cc-pVTZ	-1262.33	-1262.39	-1262.50	-1261.10	-1261.17	-1261.37	704.92	0.00
PBE0DH PBE0DH	cc-pVQZ AUG-cc-pVDZ	-1262.33 -1262.33	-1262.39 -1262.35	-1262.50 -1262.50	-1261.11 -1261.10	-1261.22 -1261.21	-1261.38 -1261.37	705.34 707.71	0.29
PBE0DH	AUG-cc-pVTZ	-1262.33	-1262.36	-1262.50	-1261.10	-1261.21	-1261.37	704.71	0.04
PBE0DH	AUG-cc-pV1Z AUG-cc-pVQZ	-1262.33	-1262.36	-1262.50	-1261.11	-1261.22	-1261.38	704.94	0.33
PBE0DH	SV	-1262.14	-1262.20	-1262.31	-1261.11	-1261.22	-1261.38	713.54	0.29
PBE0DH	SVP	-1262.14	-1262.20	-1262.31	-1260.90	-1261.01	-1261.17	713.34	0.51
PBE0DH	TZV	-1262.14	-1262.20	-1262.31	-1261.08	-1261.19	-1261.18	703.28	0.51
	TZVP								
PBE0DH	QZVP	-1262.30	-1262.36	-1262.47	-1261.08	-1261.19 -1261.22	-1261.35	703.33	0.58
PBE0DH PBE0DH	def2SV	-1262.33 -1262.14	-1262.39	-1262.50 -1262.31	-1261.11 -1260.91	-1261.22	-1261.38 -1261.18	705.20 711.01	0.31 0.51
			-1262.20						
PBE0DH PBE0DH	def2SVP def2SVPP	-1262.14 -1262.14	-1262.20 -1262.20	-1262.31 -1262.31	-1260.91 -1260.91	-1261.01 -1261.01	-1261.18 -1261.18	712.00 711.01	0.65 0.51
PBE0DH PBE0DH	def2TZV		-1262.20	-1262.31	-1261.08	-1261.01	-1261.18		0.51
		-1262.30						703.28	
PBE0DH	def2TZVP	-1262.30	-1262.36 -1262.37	-1262.48	-1261.08 -1261.09	-1261.19	-1261.35	704.12	0.47
PBE0DH	def2TZVPP def2QZV	-1262.31	-1262.37	-1262.48	-1261.09	-1261.19	-1261.35	704.63	0.39
PBE0DH		-1262.33		-1262.50		-1261.21	-1261.38	703.50	0.55
PBE0DH	def2QZVP	-1262.33	-1262.39	-1262.50	-1261.11	-1261.22	-1261.38	705.20	0.31
PBE0DH	def2QZVPP	-1262.33	-1262.39	-1262.50	-1261.11	-1261.22	-1261.38	705.29	0.30
PBEQIDH	C 21	-1248.32	-1248.62	-1248.87	-1247.46	-1247.79	-1247.99	549.34	22.35
PBEQIDH	6-31g	-1261.96	-1262.02	-1262.14	-1260.76	-1260.87	-1261.04	687.38	2.83
PBEQIDH	6-31g(d,p)	-1261.96	-1262.02	-1262.14	-1260.76	-1260.87	-1261.04	688.11	2.73
PBEQIDH	6-31+g	-1261.97	-1262.03	-1262.15	-1260.76	-1260.88	-1261.05	691.12	2.30
PBEQIDH	6-31+g(d,p)	-1261.98	-1262.04	-1262.15	-1260.77	-1260.88	-1261.05	691.82	2.20
PBEQIDH	6-31++g	-1261.97	-1262.03	-1262.15	-1260.76	-1260.88	-1261.05	691.12	2.30
PBEQIDH	6-31++g(d,p)	-1261.98	-1262.04	-1262.15	-1260.77	-1260.88	-1261.05	691.82	2.20
PBEQIDH	cc-pVDZ	-1262.14	-1262.16	-1262.31	-1260.93	-1261.00	-1261.21	694.13	1.88
PBEQIDH	cc-pVTZ	-1262.14	-1262.16	-1262.32	-1260.94	-1261.01	-1261.22	690.75	2.36
PBEQIDH	cc-pVQZ	-1262.14	-1262.20	-1262.32	-1260.94	-1261.05	-1261.22	691.15	2.30
PBEQIDH	AUG-cc-pVDZ AUG-cc-pVTZ	-1262.14	-1262.16	-1262.31	-1260.93	-1261.04	-1261.21	693.95	1.90
PBEQIDH		-1262.14	-1262.20	-1262.32	-1260.94	-1261.01	-1261.22	690.77	2.35 2.30
PBEQIDH	AUG-cc-pVQZ SV	-1262.14	-1262.20	-1262.32	-1260.94	-1261.05	-1261.22	691.15	
PBEQIDH		-1261.95	-1262.01	-1262.13	-1260.72	-1260.84	-1261.01	698.93	1.20
PBEQIDH	SVP	-1261.95	-1262.01	-1262.13	-1260.73	-1260.84	-1261.02	696.29	1.57
PBEQIDH	TZV	-1262.11	-1262.17	-1262.29	-1260.90	-1261.02	-1261.19	688.92	2.62
PBEQIDH	TZVP	-1262.11	-1262.17 -1262.20	-1262.29 -1262.32	-1260.90	-1261.02	-1261.19	688.92	2.62
PBEQIDH	QZVP	-1262.14			-1260.94	-1261.04	-1261.22	691.01	2.32
PBEQIDH	def2SV	-1261.95	-1262.01	-1262.13	-1260.73	-1260.84	-1261.02	696.29	1.57
PBEQIDH	def2SVP	-1261.95	-1262.01	-1262.13	-1260.73	-1260.84 -1260.84	-1261.02	697.55	1.39
PBEQIDH PBEQIDH	def2SVPP def2TZV	-1261.95	-1262.01 -1262.17	-1262.13 -1262.29	-1260.73 -1260.90	-1260.84	-1261.02	696.29 688.92	1.57
		-1262.11					-1261.19		2.62
PBEQIDH	def2TZVP	-1262.11	-1262.17	-1262.29	-1260.91	-1261.02	-1261.19	689.99	2.46
PBEQIDH	def2TZVPP	-1262.11	-1262.14	-1262.29	-1260.91	-1260.98	-1261.19	690.55	2.38
PBEQIDH	def2QZV	-1262.14	-1262.20	-1262.31	-1260.93	-1261.04	-1261.22 -1261.22	688.93	2.61
PBEQIDH PBEQIDH	def2QZVP def2QZVPP	-1262.14	-1262.20 -1262.20	-1262.32 -1262.32	-1260.94	-1261.04 -1261.04	-1261.22 -1261.22	691.01	2.32
MP2	ueizQZVPP	-1262.14			-1260.94	-1261.04		691.10	
MP2		-1247.69	-1247.77	-1248.07	-1246.88	-1241.28	-1247.45	387.01	45.29

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
MP2	6-31g	-1261.29	-1261.36	-1261.49	-1260.13	-1260.25	-1260.44	654.70	7.45
MP2	6-31g(d,p)	-1261.30	-1261.36	-1261.49	-1260.14	-1260.25	-1260.44	655.82	7.29
MP2	6-31+g	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	657.64	7.04
MP2	6-31+g(d,p)	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	658.73	6.88
MP2	6-31++g	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	657.64	7.04
MP2	6-31++g(d,p)	-1261.31	-1261.37	-1261.50	-1260.14	-1260.26	-1260.45	658.73	6.88
MP2	cc-pVDZ	-1261.47	-1261.50	-1261.66	-1260.30	-1260.42	-1260.61	661.75	6.46
MP2	cc-pVTZ	-1261.48	-1261.54	-1261.66	-1260.31	-1260.39	-1260.62	657.96	6.99
MP2	cc-pVQZ	-1261.48	-1261.50	-1261.67	-1260.32	-1260.43	-1260.62	658.33	6.94
MP2	AUG-cc-pVDZ	-1261.47	-1261.50	-1261.66	-1260.31	-1260.42	-1260.61	661.56	6.48
MP2	AUG-cc-pVTZ	-1261.48	-1261.54	-1261.66	-1260.31	-1260.39	-1260.62	658.00	6.99
MP2	AUG-cc-pVQZ	-1261.48	-1261.54	-1261.67	-1260.32	-1260.43	-1260.62	658.33	6.94
MP2	SV	-1261.28	-1261.34	-1261.47	-1260.10	-1260.22	-1260.41	664.79	6.03
MP2	SVP	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
MP2	TZV	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.51	7.34
MP2	TZVP	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.46	7.35
MP2	QZVP	-1261.48	-1261.54	-1261.67	-1260.31	-1260.43	-1260.62	658.18	6.96
MP2	def2SV	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
MP2	def2SVP	-1261.29	-1261.35	-1261.48	-1260.11	-1260.23	-1260.42	663.98	6.14
MP2	def2SVPP	-1261.28	-1261.35	-1261.47	-1260.11	-1260.23	-1260.42	662.11	6.40
MP2	def2TZV	-1261.44	-1261.51	-1261.63	-1260.28	-1260.40	-1260.59	655.51	7.34
MP2	def2TZVP	-1261.45	-1261.51	-1261.64	-1260.29	-1260.40	-1260.59	657.15	7.11
MP2	def2TZVPP	-1261.45	-1261.47	-1261.64	-1260.29	-1260.36	-1260.59	657.85	7.01
MP2	def2QZV	-1261.47	-1261.53	-1261.66	-1260.30	-1260.42	-1260.62	655.28	7.37
MP2	def2QZVP	-1261.48	-1261.54	-1261.67	-1260.31	-1260.43	-1260.62	658.18	6.96
MP2	def2QZVPP	-1261.48	-1261.50	-1261.67	-1260.32	-1260.39	-1260.62	658.29	6.95
OPBE	dci2@ZVII	-1248.51	-1249.34	-1249.47	-1248.39	-1248.45	-1248.59	552.67	21.87
OPBE	6-31g	-1262.57	-1262.80	-1262.89	-1240.57	-1261.54	-1261.74	716.52	1.29
OPBE	6-31g(d,p)	-1262.63	-1262.80	-1262.89	-1261.57	-1261.54	-1261.74	716.80	1.33
OPBE	6-31+g	-1262.55	-1262.82	-1262.90	-1261.58	-1261.63	-1261.75	723.12	2.22
OPBE	6-31+g(d,p)	-1262.57	-1262.82	-1262.90	-1261.58	-1261.63	-1261.75	723.39	2.26
OPBE	6-31++g	-1262.54	-1262.82	-1262.90	-1261.58	-1261.54	-1261.75	723.12	2.22
OPBE	6-31++g(d,p)	-1262.55	-1262.82	-1262.90	-1261.58	-1261.54	-1261.75	723.39	2.26
OPBE	cc-pVDZ	-1262.88	-1262.82	-1263.07	-1261.73	-1261.70	-1261.73	725.26	2.52
OPBE	cc-pVTZ	-1262.67	-1262.99	-1263.07	-1261.73	-1261.80	-1261.91	722.98	2.32
OPBE	cc-pV1Z	-1262.71	-1262.99	-1263.07	-1261.75	-1261.80	-1261.92	723.54	2.28
OPBE	AUG-cc-pVDZ	-1262.71	-1262.99	-1263.07	-1261.73	-1261.70	-1261.92	725.16	2.20
OPBE	AUG-cc-pVTZ	-1262.71	-1262.99	-1263.07	-1261.73	-1261.70	-1261.91	723.10	2.31
OPBE	AUG-cc-pV1Z	-1262.73	-1262.99	-1263.07	-1261.74	-1261.80	-1261.92	723.56	2.21
OPBE	SV	-1262.73	-1262.79	-1262.87	-1261.73	-1261.58	-1261.92	732.85	3.59
OPBE	SVP	-1262.52	-1262.79	-1262.88	-1261.53	-1261.58	-1261.71	730.15	3.21
OPBE	TZV	-1262.64	-1262.79	-1263.04	-1261.55	-1261.59	-1261.71	730.13	2.01
OPBE	TZVP		-1262.96	-1263.04	-1261.71			721.05	2.01
OPBE	QZVP	-1262.71 -1262.84	-1262.96	-1263.04	-1261.71	-1261.77 -1261.80	-1261.89 -1261.92	723.22	2.03
OPBE	def2SV	-1262.84	-1262.98	-1263.07	-1261.74	-1261.80	-1261.92	730.15	3.21
OPBE	def2SVP							730.13	
OPBE		-1262.51	-1262.80	-1262.88	-1261.53	-1261.59	-1261.71		3.29
	def2SVPP	-1262.56	-1262.79	-1262.88	-1261.53	-1261.50	-1261.71	730.15	3.21
OPBE	def2TZV	-1262.68	-1262.96	-1263.04	-1261.71	-1261.77	-1261.89	721.65	2.01
OPBE	def2TZVP	-1262.81	-1262.96	-1263.04	-1261.71	-1261.77	-1261.89	722.38	2.12
OPBE	def2TZVPP	-1262.72	-1262.96	-1263.04	-1261.72	-1261.77	-1261.89	722.82	2.18
OPBE	def2QZV	-1262.89	-1262.99	-1263.07	-1261.74	-1261.70	-1261.92	722.14	2.08

Table 1: Datos de los funcionales y funciones base exploradas para el calculo de la 3EI en Hartrees

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
OPBE	def2QZVP	-1262.84	-1262.98	-1263.07	-1261.74	-1261.80	-1261.92	723.22	2.23
OPBE	def2QZVPP	-1262.70	-1262.98	-1263.07	-1261.74	-1261.80	-1261.92	723.31	2.25