

Anexo 1

Adrian Leonardo Orjuela Rocha

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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-pVQZ	-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	-1262.49	-1262.54	-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	-1262.74	-1262.83	-1261.43	-1261.53	-1261.67	728.47	2.98
B3LYP	def2SV	-1262.49	-1262.54	-1262.63	-1261.23	-1261.32	-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	-1262.49	-1262.54	-1262.63	-1261.23	-1261.32	-1261.46	734.54	3.83
B3LYP	def2TZV	-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

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Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
O3LYP	6-31g	-1262.65	-1262.70	-1262.82	-1261.42	-1261.56	-1261.67	716.36	1.26
O3LYP	6-31g(d,p)	-1262.65	-1262.70	-1262.82	-1261.42	-1261.56	-1261.67	716.65	1.30
O3LYP	6-31+g	-1262.67	-1262.72	-1262.83	-1261.45	-1261.56	-1261.68	723.27	2.24
O3LYP	6-31+g(d,p)	-1262.67	-1262.72	-1262.83	-1261.45	-1261.56	-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
O3LYP	6-31++g(d,p)	-1262.67	-1262.72	-1262.83	-1261.45	-1261.56	-1261.68	723.55	2.28
O3LYP	cc-pVDZ	-1262.83	-1262.88	-1263.00	-1261.59	-1261.72	-1261.84	725.41	2.54
O3LYP	cc-pVTZ	-1262.83	-1262.88	-1263.00	-1261.62	-1261.73	-1261.85	723.40	2.26
O3LYP	cc-pVQZ	-1262.84	-1262.89	-1263.00	-1261.62	-1261.73	-1261.85	723.59	2.29
O3LYP	AUG-cc-pVDZ	-1262.83	-1262.88	-1263.00	-1261.59	-1261.72	-1261.84	725.32	2.53
O3LYP	AUG-cc-pVTZ	-1262.83	-1262.88	-1263.00	-1261.62	-1261.73	-1261.85	723.43	2.26
O3LYP	AUG-cc-pVQZ	-1262.84	-1262.89	-1263.00	-1261.62	-1261.73	-1261.85	723.85	2.32
O3LYP	SV	-1262.64	-1262.69	-1262.81	-1261.38	-1261.52	-1261.64	732.78	3.59
O3LYP	SVP	-1262.64	-1262.69	-1262.81	-1261.38	-1261.52	-1261.64	730.48	3.26
O3LYP	TZV	-1262.81	-1262.86	-1262.97	-1261.59	-1261.70	-1261.82	721.99	2.06
O3LYP	TZVP	-1262.81	-1262.86	-1262.97	-1261.59	-1261.70	-1261.82	722.17	2.08
O3LYP	QZVP	-1262.83	-1262.89	-1263.00	-1261.62	-1261.73	-1261.85	723.51	2.27
O3LYP	def2SV	-1262.64	-1262.69	-1262.81	-1261.38	-1261.52	-1261.64	730.17	3.22
O3LYP	def2SVP	-1262.64	-1262.69	-1262.81	-1261.38	-1261.52	-1261.64	730.76	3.30
O3LYP	def2SVPP	-1262.64	-1262.69	-1262.81	-1261.38	-1261.52	-1261.64	730.17	3.22
O3LYP	def2TZV	-1262.81	-1262.86	-1262.97	-1261.59	-1261.70	-1261.82	721.99	2.06
O3LYP	def2TZVP	-1262.81	-1262.86	-1262.97	-1261.59	-1261.70	-1261.82	722.71	2.16
O3LYP	def2TZVPP	-1262.81	-1262.86	-1262.97	-1261.57	-1261.71	-1261.82	722.87	2.18
O3LYP	def2QZV	-1262.83	-1262.88	-1263.00	-1261.62	-1261.73	-1261.85	722.70	2.16
O3LYP	def2QZVP	-1262.83	-1262.89	-1263.00	-1261.62	-1261.73	-1261.85	723.51	2.27
O3LYP	def2QZVPP	-1262.83	-1262.89	-1263.00	-1261.62	-1261.73	-1261.85	723.84	2.32
APFD		-1248.72	-1248.84	-1249.05	-1247.91	-1247.98	-1248.16	554.79	21.58
APFD	6-31g	-1262.33	-1262.29	-1262.49	-1261.13	-1261.20	-1261.35	715.59	1.15
APFD	6-31g(d,p)	-1262.33	-1262.29	-1262.49	-1261.14	-1261.20	-1261.35	715.95	1.21
APFD	6-31+g	-1262.34	-1262.39	-1262.50	-1261.11	-1261.25	-1261.35	721.76	2.03
APFD	6-31+g(d,p)	-1262.34	-1262.39	-1262.50	-1261.11	-1261.25	-1261.35	722.11	2.08
APFD	6-31++g	-1262.34	-1262.39	-1262.50	-1261.11	-1261.25	-1261.35	721.76	2.03
APFD	6-31++g(d,p)	-1262.34	-1262.39	-1262.50	-1261.11	-1261.25	-1261.35	722.11	2.08
APFD	cc-pVDZ	-1262.51	-1262.56	-1262.67	-1261.27	-1261.41	-1261.51	723.51	2.27
APFD	cc-pVTZ	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	720.98	1.92
APFD	cc-pVQZ	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	721.90	2.05
APFD	AUG-cc-pVDZ	-1262.51	-1262.56	-1262.66	-1261.27	-1261.41	-1261.51	722.89	2.19
APFD	AUG-cc-pVTZ	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	721.00	1.92
APFD	AUG-cc-pVQZ	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	721.43	1.98
APFD	SV	-1262.32	-1262.36	-1262.48	-1261.07	-1261.20	-1261.31	730.26	3.23
APFD	SVP	-1262.32	-1262.37	-1262.48	-1261.07	-1261.21	-1261.32	727.91	2.90
APFD	TZV	-1262.48	-1262.53	-1262.64	-1261.25	-1261.39	-1261.49	719.82	1.75
APFD	TZVP	-1262.48	-1262.53	-1262.64	-1261.25	-1261.39	-1261.49	719.95	1.77
APFD	QZVP	-1262.51	-1262.56	-1262.67	-1261.28	-1261.42	-1261.52	721.76	2.03
APFD	def2SV	-1262.32	-1262.37	-1262.48	-1261.07	-1261.21	-1261.32	727.41	2.83
APFD	def2SVP	-1262.32	-1262.37	-1262.48	-1261.07	-1261.21	-1261.32	728.62	3.00
APFD	def2SVPP	-1262.32	-1262.37	-1262.48	-1261.07	-1261.21	-1261.32	727.41	2.83
APFD	def2TZV	-1262.48	-1262.53	-1262.64	-1261.25	-1261.39	-1261.49	719.82	1.75
APFD	def2TZVP	-1262.48	-1262.53	-1262.64	-1261.25	-1261.39	-1261.49	720.45	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

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Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
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	-1261.28	-1261.42	-1261.52	721.85	2.04
wB97XD		-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	-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
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
LC-wHPBE		-1248.52	-1248.74	-1248.93	-1247.80	-1247.94	-1248.05	552.94	21.84
LC-wHPBE	6-31g	-1262.27	-1262.32	-1262.42	-1261.04	-1261.18	-1261.27	720.80	1.89
LC-wHPBE	6-31g(d,p)	-1262.27	-1262.32	-1262.42	-1261.04	-1261.09	-1261.27	721.11	1.94
LC-wHPBE	6-31+g	-1262.29	-1262.33	-1262.44	-1261.05	-1261.10	-1261.28	728.06	2.92
LC-wHPBE	6-31+g(d,p)	-1262.29	-1262.33	-1262.44	-1261.05	-1261.10	-1261.28	728.36	2.96
LC-wHPBE	6-31++g	-1262.29	-1262.33	-1262.44	-1261.05	-1261.09	-1261.28	728.06	2.92
LC-wHPBE	6-31++g(d,p)	-1262.29	-1262.33	-1262.44	-1261.05	-1261.10	-1261.28	728.36	2.96
LC-wHPBE	cc-pVDZ	-1262.45	-1262.50	-1262.60	-1261.21	-1261.25	-1261.44	730.00	3.19
LC-wHPBE	cc-pVTZ	-1262.45	-1262.50	-1262.60	-1261.21	-1261.27	-1261.44	727.86	2.89
LC-wHPBE	cc-pVQZ	-1262.45	-1262.50	-1262.61	-1261.22	-1261.35	-1261.45	728.29	2.95
LC-wHPBE	AUG-cc-pVDZ	-1262.45	-1262.50	-1262.60	-1261.21	-1261.34	-1261.44	729.91	3.18
LC-wHPBE	AUG-cc-pVTZ	-1262.45	-1262.50	-1262.60	-1261.21	-1261.27	-1261.44	727.89	2.89
LC-wHPBE	AUG-cc-pVQZ	-1262.45	-1262.50	-1262.61	-1261.22	-1261.27	-1261.45	728.78	3.02
LC-wHPBE	SV	-1262.26	-1262.30	-1262.41	-1261.00	-1261.05	-1261.24	735.86	4.02
LC-wHPBE	SVP	-1262.26	-1262.31	-1262.41	-1261.01	-1261.06	-1261.24	734.12	3.77
LC-wHPBE	TZV	-1262.42	-1262.47	-1262.58	-1261.19	-1261.32	-1261.42	726.55	2.70
LC-wHPBE	TZVP	-1262.42	-1262.47	-1262.58	-1261.19	-1261.32	-1261.42	726.86	2.75
LC-wHPBE	QZVP	-1262.45	-1262.50	-1262.61	-1261.21	-1261.27	-1261.45	728.67	3.00
LC-wHPBE	def2SV	-1262.26	-1262.31	-1262.41	-1261.01	-1261.15	-1261.24	733.56	3.70
LC-wHPBE	def2SVP	-1262.26	-1262.31	-1262.41	-1261.01	-1261.15	-1261.24	734.19	3.78
LC-wHPBE	def2SVPP	-1262.26	-1262.31	-1262.41	-1261.01	-1261.06	-1261.24	733.56	3.70
LC-wHPBE	def2TZV	-1262.42	-1262.47	-1262.57	-1261.19	-1261.23	-1261.42	726.02	2.63

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
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		-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	-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

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-pVQZ	-1262.56	-1262.62	-1262.72	-1261.33	-1261.44	-1261.57	723.66	2.30
M11	AUG-cc-pVDZ	-1262.55	-1262.61	-1262.71	-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	2.23
M11	AUG-cc-pVQZ	-1262.56	-1262.62	-1262.72	-1261.33	-1261.44	-1261.57	723.66	2.30
M11	SV	-1262.35	-1262.42	-1262.51	-1261.11	-1261.22	-1261.35	728.98	3.05
M11	SVP	-1262.35	-1262.42	-1262.51	-1261.12	-1261.23	-1261.36	727.24	2.80
M11	TZV	-1262.52	-1262.58	-1262.68	-1261.30	-1261.40	-1261.53	720.81	1.89

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		-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	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	def2TZVP	-1262.56	-1262.59	-1262.64	-1261.32	-1261.39	-1261.49	725.01	2.49
MN12SX	def2TZVPP	-1262.56	-1262.59	-1262.65	-1261.33	-1261.34	-1261.49	725.57	2.57
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	def2QZVPP	-1262.60	-1262.63	-1262.69	-1261.36	-1261.43	-1261.53	725.96	2.62
PW6B95		-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	-1258.30	-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(d,p)	-1233.19	-1263.25	-1258.30	-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	-1262.12	-1262.25	-1262.36	724.18	2.37
PW6B95	cc-pVQZ	-1263.37	-1263.42	-1263.51	-1262.12	-1262.22	-1262.36	724.61	2.43

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
PW6B95	AUG-cc-pVDZ	-1263.36	-1252.98	-1255.64	-1259.76	-1256.85	-1262.35	634.31	10.34
PW6B95	AUG-cc-pVTZ	-1263.36	-1263.42	-1263.51	-1262.12	-1262.21	-1262.36	724.19	2.37
PW6B95	AUG-cc-pVQZ	-1263.37	-1263.42	-1263.51	-1262.12	-1262.22	-1262.36	724.60	2.43
PW6B95	SV	-1263.17	-1262.56	-1263.32	-1261.95	-1262.04	-1262.15	733.44	3.68
PW6B95	SVP	-1263.17	-1263.22	-1263.32	-1261.91	-1262.01	-1262.15	731.15	3.35
PW6B95	TZV	-1263.34	-1263.39	-1263.48	-1262.09	-1262.19	-1262.33	722.54	2.14
PW6B95	TZVP	-1263.34	-1263.39	-1263.48	-1262.09	-1262.19	-1262.33	722.72	2.16
PW6B95	QZVP	-1263.36	-1260.83	-1250.04	-1262.12	-1262.26	-1262.36	632.50	10.59
PW6B95	def2SV	-1263.17	-1263.22	-1263.32	-1261.91	-1262.01	-1262.15	731.15	3.35
PW6B95	def2SVP	-1263.17	-1263.23	-1263.32	-1261.91	-1262.01	-1262.15	731.79	3.45
PW6B95	def2SVPP	-1263.17	-1263.22	-1263.32	-1261.91	-1262.01	-1262.15	731.15	3.35
PW6B95	def2TZV	-1263.34	-1263.39	-1263.48	-1262.09	-1262.19	-1262.33	722.54	2.14
PW6B95	def2TZVP	-1263.34	-1263.39	-1263.48	-1262.09	-1262.19	-1262.33	723.18	2.23
PW6B95	def2TZVPP	-1263.34	-1263.39	-1263.48	-1262.10	-1260.48	-1262.33	723.63	2.29
PW6B95	def2QZV	-1263.36	-1263.42	-1263.51	-1262.12	-1262.21	-1262.36	723.49	2.27
PW6B95	def2QZVP	-1263.36	-1263.45	-1250.04	-1262.12	-1262.21	-1262.36	685.22	3.14
PW6B95	def2QZVPP	-1263.36	-1263.45	-1263.51	-1262.12	-1262.26	-1262.36	724.50	2.41
M08HX		-1248.66	-1248.88	-1249.11	-1247.97	-1248.06	-1248.23	556.66	21.31
M08HX	6-31g	-1262.43	-1262.49	-1262.59	-1261.21	-1261.32	-1261.46	706.74	0.10
M08HX	6-31g(d,p)	-1262.43	-1262.49	-1262.59	-1261.21	-1261.32	-1261.46	707.00	0.06
M08HX	6-31+g	-1262.45	-1262.51	-1262.60	-1261.22	-1261.32	-1261.47	714.08	0.94
M08HX	6-31+g(d,p)	-1262.45	-1262.51	-1262.60	-1261.22	-1261.33	-1261.47	714.33	0.98
M08HX	6-31++g	-1262.45	-1262.51	-1262.60	-1261.22	-1261.32	-1261.47	714.08	0.94
M08HX	6-31++g(d,p)	-1262.45	-1262.51	-1262.60	-1261.22	-1261.33	-1261.47	714.33	0.98
M08HX	cc-pVDZ	-1262.62	-1262.63	-1262.78	-1261.39	-1261.44	-1261.64	715.13	1.09
M08HX	cc-pVTZ	-1262.62	-1262.64	-1262.78	-1261.40	-1261.50	-1261.64	713.13	0.81
M08HX	cc-pVQZ	-1262.63	-1262.69	-1262.78	-1261.40	-1261.51	-1261.65	713.66	0.88
M08HX	AUG-cc-pVDZ	-1262.62	-1262.63	-1262.78	-1261.39	-1261.44	-1261.64	715.05	1.08
M08HX	AUG-cc-pVTZ	-1262.62	-1262.68	-1262.78	-1261.40	-1261.50	-1261.64	713.14	0.81
M08HX	AUG-cc-pVQZ	-1262.63	-1262.69	-1262.78	-1261.40	-1261.45	-1261.65	713.67	0.88
M08HX	SV	-1262.43	-1262.49	-1262.59	-1261.19	-1261.30	-1261.44	719.94	1.77
M08HX	SVP	-1262.43	-1262.49	-1262.59	-1261.19	-1261.30	-1261.45	718.01	1.50
M08HX	TZV	-1262.59	-1262.66	-1262.75	-1261.37	-1261.48	-1261.62	711.57	0.59
M08HX	TZVP	-1262.59	-1262.66	-1262.75	-1261.37	-1261.48	-1261.62	711.68	0.60
M08HX	QZVP	-1262.63	-1262.69	-1262.78	-1261.40	-1261.51	-1261.65	713.41	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
M06	6-31g(d,p)	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.45	704.30	0.44
M06	6-31+g	-1262.43	-1262.49	-1262.58	-1261.17	-1261.28	-1261.45	711.07	0.52
M06	6-31+g(d,p)	-1262.43	-1262.49	-1262.58	-1261.17	-1261.28	-1261.45	711.28	0.55
M06	6-31++g	-1262.43	-1262.49	-1262.58	-1261.17	-1261.28	-1261.45	711.07	0.52
M06	6-31++g(d,p)	-1262.43	-1262.49	-1262.58	-1261.17	-1261.28	-1261.45	711.28	0.55

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
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	0.23
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	706.94	0.07
M06	def2QZVPP	-1262.59	-1262.65	-1262.74	-1261.34	-1261.45	-1261.62	706.99	0.06
M062X		-1248.72	-1248.94	-1249.17	-1247.82	-1248.10	-1248.28	561.60	20.61
M062X	6-31g	-1262.44	-1262.50	-1262.59	-1261.21	-1261.32	-1261.46	711.03	0.51
M062X	6-31g(d,p)	-1262.44	-1262.50	-1262.59	-1261.21	-1261.32	-1261.46	711.33	0.55
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	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
M05	6-31g(d,p)	-1262.48	-1262.54	-1262.65	-1261.23	-1261.35	-1261.53	702.97	0.63
M05	6-31+g	-1262.49	-1262.56	-1262.67	-1261.24	-1261.36	-1261.53	710.05	0.37

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		-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-pVQZ	-1262.58	-1262.65	-1262.75	-1261.36	-1261.47	-1261.61	714.49	1.00
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	SV	-1262.39	-1262.45	-1262.56	-1261.15	-1261.26	-1261.41	720.70	1.88
M052X	SVP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.26	-1261.42	719.00	1.64
M052X	TZV	-1262.55	-1262.61	-1262.72	-1261.32	-1261.44	-1261.58	711.62	0.59
M052X	TZVP	-1262.55	-1262.61	-1262.72	-1261.32	-1261.44	-1261.58	711.85	0.63
M052X	QZVP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.47	-1261.61	714.43	0.99
M052X	def2SV	-1262.39	-1262.46	-1262.56	-1261.15	-1261.26	-1261.42	719.00	1.64
M052X	def2SVP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.27	-1261.42	719.60	1.72
M052X	def2SVPP	-1262.39	-1262.46	-1262.56	-1261.15	-1261.26	-1261.42	719.00	1.64
M052X	def2TZV	-1262.55	-1262.61	-1262.72	-1261.32	-1261.44	-1261.58	711.62	0.59
M052X	def2TZVP	-1262.55	-1262.61	-1262.72	-1261.33	-1261.44	-1261.58	712.27	0.69
M052X	def2TZVPP	-1262.55	-1262.61	-1262.72	-1261.33	-1261.44	-1261.58	712.72	0.75
M052X	def2QZV	-1262.58	-1262.64	-1262.75	-1261.35	-1261.46	-1261.61	713.29	0.83
M052X	def2QZVP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.47	-1261.61	714.43	0.99
M052X	def2QZVPP	-1262.58	-1262.64	-1262.75	-1261.36	-1261.47	-1261.61	714.51	1.00
PBE1PBE		-1248.65	-1248.86	-1248.98	-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

Functional	Basis set	1	3	5	2	4	6	3IE Kcal/mol	%Error
PBE1PBE	6-31g	-1262.24	-1262.30	-1262.41	-1261.01	-1261.12	-1261.27	713.77	0.90
PBE1PBE	6-31g(d,p)	-1262.24	-1262.30	-1262.41	-1261.01	-1261.12	-1261.27	714.13	0.95
PBE1PBE	6-31+g	-1262.26	-1262.32	-1262.42	-1261.02	-1261.12	-1261.27	719.91	1.77
PBE1PBE	6-31+g(d,p)	-1262.26	-1262.32	-1262.42	-1261.02	-1261.12	-1261.27	720.27	1.82
PBE1PBE	6-31++g	-1262.26	-1262.32	-1262.42	-1261.02	-1261.12	-1261.27	719.91	1.77
PBE1PBE	6-31++g(d,p)	-1262.26	-1262.32	-1262.42	-1261.02	-1261.12	-1261.27	720.27	1.82
PBE1PBE	cc-pVDZ	-1262.42	-1262.48	-1262.58	-1261.18	-1261.28	-1261.43	721.54	2.00
PBE1PBE	cc-pVTZ	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.38	1.69
PBE1PBE	cc-pVQZ	-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	719.79	1.75
PBE1PBE	AUG-cc-pVDZ	-1262.42	-1262.44	-1262.58	-1261.18	-1261.28	-1261.43	721.41	1.98
PBE1PBE	AUG-cc-pVTZ	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.40	1.69
PBE1PBE	AUG-cc-pVQZ	-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	719.79	1.75
PBE1PBE	SV	-1262.23	-1262.29	-1262.39	-1260.98	-1261.08	-1261.23	728.10	2.92
PBE1PBE	SVP	-1262.23	-1262.29	-1262.39	-1260.98	-1261.08	-1261.24	725.77	2.59
PBE1PBE	TZV	-1262.40	-1262.45	-1262.56	-1261.16	-1261.26	-1261.41	717.79	1.47
PBE1PBE	TZVP	-1262.40	-1262.46	-1262.56	-1261.16	-1261.26	-1261.41	717.92	1.48
PBE1PBE	QZVP	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.67	1.73
PBE1PBE	def2SV	-1262.23	-1262.29	-1262.39	-1260.98	-1261.08	-1261.24	725.77	2.59
PBE1PBE	def2SVP	-1262.23	-1262.29	-1262.40	-1260.98	-1261.08	-1261.24	726.50	2.70
PBE1PBE	def2SVPP	-1262.23	-1262.29	-1262.39	-1260.98	-1261.08	-1261.24	725.77	2.59
PBE1PBE	def2TZV	-1262.40	-1262.45	-1262.56	-1261.16	-1261.26	-1261.41	717.79	1.47
PBE1PBE	def2TZVP	-1262.40	-1262.46	-1262.56	-1261.16	-1261.26	-1261.41	718.46	1.56
PBE1PBE	def2TZVPP	-1262.40	-1262.46	-1262.56	-1261.16	-1261.26	-1261.41	718.94	1.63
PBE1PBE	def2QZV	-1262.42	-1262.48	-1262.59	-1261.18	-1261.29	-1261.44	718.34	1.54
PBE1PBE	def2QZVP	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.67	1.73
PBE1PBE	def2QZVPP	-1262.42	-1262.48	-1262.59	-1261.19	-1261.29	-1261.44	719.76	1.74
HSEH1PBE		-1248.67	-1248.88	-1249.00	-1247.86	-1247.94	-1248.12	554.89	21.56
HSEH1PBE	6-31g	-1262.26	-1262.31	-1262.42	-1261.03	-1261.13	-1261.28	714.36	0.98
HSEH1PBE	6-31g(d,p)	-1262.26	-1262.31	-1262.42	-1261.03	-1261.13	-1261.28	714.72	1.03
HSEH1PBE	6-31+g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.52	1.85
HSEH1PBE	6-31+g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.87	1.90
HSEH1PBE	6-31++g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.52	1.85
HSEH1PBE	6-31++g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.87	1.90
HSEH1PBE	cc-pVDZ	-1262.43	-1262.49	-1262.59	-1261.19	-1261.29	-1261.44	722.25	2.10
HSEH1PBE	cc-pVTZ	-1262.44	-1262.46	-1262.60	-1261.20	-1261.30	-1261.45	720.03	1.78
HSEH1PBE	cc-pVQZ	-1262.44	-1262.46	-1262.60	-1261.20	-1261.30	-1261.45	720.38	1.83
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	-1262.31	-1262.41	-1261.00	-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	719.14	1.66
HSEH1PBE	def2TZVPP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	719.62	1.72
HSEH1PBE	def2QZV	-1262.44	-1262.49	-1262.60	-1261.20	-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 Kcal/mol	%Error
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		-1248.95	-1249.15	-1249.27	-1248.13	-1248.20	-1248.38	560.07	20.83
OHSE2PBE	6-31g	-1262.53	-1262.59	-1262.69	-1261.29	-1261.39	-1261.54	721.24	1.95
OHSE2PBE	6-31g(d,p)	-1262.53	-1262.59	-1262.69	-1261.29	-1261.39	-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 Kcal/mol	%Error
B98	def2TZVP	-1262.59	-1262.63	-1262.74	-1261.36	-1261.48	-1261.58	721.92	2.05
B98	def2TZVPP	-1262.59	-1262.64	-1262.74	-1261.36	-1261.48	-1261.59	722.34	2.11
B98	def2QZV	-1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	722.01	2.06
B98	def2QZVP	-1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	723.17	2.23
B98	def2QZVPP	-1262.62	-1262.66	-1262.76	-1261.39	-1261.51	-1261.61	722.95	2.19
B972		-1249.14	-1249.25	-1249.46	-1248.32	-1248.44	-1248.58	550.22	22.22
B972	6-31g	-1262.72	-1262.77	-1262.88	-1261.49	-1261.62	-1261.74	715.34	1.12
B972	6-31g(d,p)	-1262.72	-1262.77	-1262.88	-1261.49	-1261.62	-1261.74	715.61	1.16
B972	6-31+g	-1262.74	-1262.78	-1262.89	-1261.50	-1261.63	-1261.74	721.06	1.93
B972	6-31+g(d,p)	-1262.74	-1262.78	-1262.89	-1261.50	-1261.63	-1261.74	721.33	1.97
B972	6-31++g	-1262.74	-1262.78	-1262.89	-1261.50	-1261.63	-1261.74	721.06	1.93
B972	6-31++g(d,p)	-1262.74	-1262.78	-1262.89	-1261.50	-1261.55	-1261.74	721.33	1.97
B972	cc-pVDZ	-1262.90	-1262.95	-1263.05	-1261.66	-1261.79	-1261.90	721.86	2.04
B972	cc-pVTZ	-1262.90	-1262.95	-1263.06	-1261.67	-1261.72	-1261.91	719.61	1.72
B972	cc-pVQZ	-1262.91	-1262.95	-1263.06	-1261.67	-1261.72	-1261.91	720.53	1.85
B972	AUG-cc-pVDZ	-1262.90	-1262.95	-1263.05	-1261.66	-1261.71	-1261.90	722.01	2.06
B972	AUG-cc-pVTZ	-1262.90	-1262.95	-1263.06	-1261.67	-1261.72	-1261.91	719.62	1.73
B972	AUG-cc-pVQZ	-1262.91	-1262.95	-1263.06	-1261.67	-1261.72	-1261.91	720.37	1.83
B972	SV	-1262.71	-1262.75	-1262.86	-1261.45	-1261.59	-1261.70	728.59	2.99
B972	SVP	-1262.71	-1262.76	-1262.87	-1261.46	-1261.59	-1261.71	726.05	2.63
B972	TZV	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.48	1.56
B972	TZVP	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.62	1.58
B972	QZVP	-1262.90	-1262.95	-1263.06	-1261.67	-1261.72	-1261.91	719.97	1.77
B972	def2SV	-1262.71	-1262.76	-1262.86	-1261.46	-1261.51	-1261.71	725.78	2.60
B972	def2SVP	-1262.71	-1262.76	-1262.87	-1261.46	-1261.59	-1261.71	726.40	2.68
B972	def2SVPP	-1262.71	-1262.76	-1262.86	-1261.46	-1261.51	-1261.71	725.78	2.60
B972	def2TZV	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.23	1.53
B972	def2TZVP	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	718.91	1.62
B972	def2TZVPP	-1262.88	-1262.92	-1263.03	-1261.64	-1261.77	-1261.88	719.51	1.71
B972	def2QZV	-1262.90	-1262.95	-1263.06	-1261.67	-1261.79	-1261.91	719.09	1.65
B972	def2QZVP	-1262.90	-1262.95	-1263.06	-1261.67	-1261.80	-1261.91	720.19	1.80
B972	def2QZVPP	-1262.90	-1262.95	-1263.06	-1261.67	-1261.80	-1261.91	720.24	1.81
OHSEIPBE		-1248.67	-1248.88	-1249.00	-1247.87	-1247.90	-1248.12	554.89	21.56
OHSEIPBE	6-31g	-1262.26	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	714.36	0.98
OHSEIPBE	6-31g(d,p)	-1262.26	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	714.72	1.03
OHSEIPBE	6-31+g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.53	1.85
OHSEIPBE	6-31+g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.88	1.90
OHSEIPBE	6-31++g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.53	1.85
OHSEIPBE	6-31++g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.28	720.88	1.90
OHSEIPBE	cc-pVDZ	-1262.43	-1262.46	-1262.60	-1261.19	-1261.29	-1261.44	722.26	2.10
OHSEIPBE	cc-pVTZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.03	1.78
OHSEIPBE	cc-pVQZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.27	-1261.45	720.39	1.83
OHSEIPBE	AUG-cc-pVDZ	-1262.43	-1262.46	-1262.60	-1261.19	-1261.29	-1261.44	722.13	2.08
OHSEIPBE	AUG-cc-pVTZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.05	1.79
OHSEIPBE	AUG-cc-pVQZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.39	1.83
OHSEIPBE	SV	-1262.25	-1262.30	-1262.41	-1260.99	-1261.09	-1261.24	728.66	3.00
OHSEIPBE	SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	726.34	2.67
OHSEIPBE	TZV	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	718.49	1.56
OHSEIPBE	TZVP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	718.62	1.58
OHSEIPBE	QZVP	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.32	1.82
OHSEIPBE	def2SV	-1262.25	-1262.31	-1262.41	-1261.00	-1261.06	-1261.25	726.34	2.67

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
OHSE1PBE	def2SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	727.06	2.78
OHSE1PBE	def2SVPP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	726.34	2.67
OHSE1PBE	def2TZV	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.42	718.49	1.56
OHSE1PBE	def2TZVP	-1262.41	-1262.47	-1262.57	-1261.17	-1261.27	-1261.43	719.14	1.66
OHSE1PBE	def2TZVPP	-1262.41	-1262.47	-1262.57	-1261.18	-1261.27	-1261.43	719.63	1.73
OHSE1PBE	def2QZV	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	718.99	1.64
OHSE1PBE	def2QZVP	-1262.44	-1262.50	-1262.60	-1261.20	-1261.27	-1261.45	720.32	1.82
OHSE1PBE	def2QZVPP	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.40	1.84
PBEh1PBE		-1248.67	-1248.88	-1249.00	-1247.87	-1247.94	-1248.12	554.95	21.55
PBEh1PBE	6-31g	-1262.26	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	714.35	0.98
PBEh1PBE	6-31g(d,p)	-1262.26	-1262.32	-1262.42	-1261.03	-1261.13	-1261.28	714.72	1.03
PBEh1PBE	6-31+g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.29	720.55	1.86
PBEh1PBE	6-31+g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.29	720.90	1.90
PBEh1PBE	6-31++g	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.29	720.55	1.86
PBEh1PBE	6-31++g(d,p)	-1262.27	-1262.33	-1262.43	-1261.03	-1261.13	-1261.29	720.90	1.90
PBEh1PBE	cc-pVDZ	-1262.44	-1262.46	-1262.60	-1261.19	-1261.29	-1261.45	722.27	2.10
PBEh1PBE	cc-pVTZ	-1262.44	-1262.46	-1262.60	-1261.20	-1261.30	-1261.45	720.04	1.78
PBEh1PBE	cc-pVQZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.40	1.83
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	-1262.46	-1262.60	-1261.20	-1261.30	-1261.45	720.06	1.79
PBEh1PBE	AUG-cc-pVQZ	-1262.44	-1262.50	-1262.60	-1261.20	-1261.30	-1261.45	720.40	1.83
PBEh1PBE	SV	-1262.25	-1262.31	-1262.41	-1260.99	-1261.09	-1261.25	728.64	3.00
PBEh1PBE	SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	726.33	2.67
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	-1261.10	-1261.25	726.33	2.67
PBEh1PBE	def2SVP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.10	-1261.25	727.05	2.77
PBEh1PBE	def2SVPP	-1262.25	-1262.31	-1262.41	-1261.00	-1261.06	-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	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	720.41	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	-1262.68	-1260.66	-1262.83	-1222.19	-1261.57	-1261.68	720.73	1.88
B1B95	6-31++g(d,p)	-1232.86	-1256.24	-1262.83	-1222.21	-1239.75	-1261.68	721.05	1.93
B1B95	cc-pVDZ	-1262.84	-1262.85	-1249.66	-1261.60	-1249.72	-1248.46	789.01	11.53
B1B95	cc-pVTZ	-1262.84	-1262.90	-1262.99	-1241.51	-1261.74	-1261.85	719.33	1.68
B1B95	cc-pVQZ	-1262.84	-1260.38	-1263.00	-1261.61	-1261.70	-1261.85	719.74	1.74
B1B95	AUG-cc-pVDZ	-1262.84	-1260.62	-1262.99	-1261.60	-1261.73	-1237.56	787.87	11.37
B1B95	AUG-cc-pVTZ	-1262.84	-1262.90	-1262.99	-1261.69	-1251.69	-1261.85	719.34	1.69
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
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		-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-pVQZ	-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	724.68	2.44
TPSSh	SV	-1262.48	-1262.53	-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	-1262.65	-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	2.15
TPSSh	QZVP	-1262.67	-1262.73	-1262.82	-1261.44	-1261.53	-1261.67	724.46	2.41
TPSSh	def2SV	-1262.48	-1262.54	-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		-1248.40	-1249.02	-1249.14	-1248.02	-1248.09	-1248.26	553.21	21.80
tHCTHhyb	6-31g	-1262.49	-1262.54	-1262.63	-1261.24	-1261.34	-1261.48	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(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	-1261.52	-1261.66	726.75	2.73
tHCTHhyb	cc-pVQZ	-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	-1261.51	-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

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
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	713.90	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		-1248.65	-1248.86	-1248.97	-1247.85	-1247.92	-1248.09	551.99	21.97
HISSbPBE	6-31g	-1262.29	-1262.34	-1262.44	-1261.07	-1261.20	-1261.30	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	2.28
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	2.28
HISSbPBE	cc-pVDZ	-1262.46	-1262.51	-1262.62	-1261.23	-1261.37	-1261.47	724.83	2.46
HISSbPBE	cc-pVTZ	-1262.47	-1262.52	-1262.62	-1261.24	-1261.29	-1261.47	722.61	2.15
HISSbPBE	cc-pVQZ	-1262.47	-1262.52	-1262.63	-1261.24	-1261.38	-1261.48	723.50	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
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		-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(d,p)	-1262.44	-1262.49	-1262.58	-1261.19	-1261.29	-1261.43	726.97	2.76
X3LYP	cc-pVDZ	-1262.60	-1262.65	-1262.75	-1261.35	-1261.45	-1261.59	727.55	2.84
X3LYP	cc-pVTZ	-1262.60	-1262.66	-1262.75	-1261.36	-1261.45	-1261.59	726.08	2.64
X3LYP	cc-pVQZ	-1262.61	-1262.66	-1262.75	-1261.36	-1261.46	-1261.60	726.42	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 Kcal/mol	%Error
BHandH	cc-pVDZ	-1260.85	-1260.91	-1261.02	-1259.62	-1259.73	-1259.89	706.76	0.09
BHandH	cc-pVTZ	-1260.85	-1260.88	-1261.02	-1259.63	-1259.74	-1259.90	704.49	0.41
BHandH	cc-pVQZ	-1260.86	-1260.88	-1261.03	-1259.63	-1259.74	-1259.90	704.86	0.36
BHandH	AUG-cc-pVDZ	-1260.85	-1260.87	-1261.02	-1259.62	-1259.73	-1259.90	706.62	0.11
BHandH	AUG-cc-pVTZ	-1260.85	-1260.88	-1261.02	-1259.63	-1259.74	-1259.90	704.50	0.41
BHandH	AUG-cc-pVQZ	-1260.86	-1260.92	-1261.03	-1259.63	-1259.74	-1259.90	704.85	0.36
BHandH	SV	-1260.66	-1260.68	-1260.83	-1259.42	-1259.53	-1259.70	712.40	0.70
BHandH	SVP	-1260.66	-1260.72	-1260.83	-1259.43	-1259.54	-1259.70	710.37	0.42
BHandH	TZV	-1260.83	-1260.89	-1260.99	-1259.60	-1259.71	-1259.87	702.87	0.64
BHandH	TZVP	-1260.83	-1260.89	-1261.00	-1259.60	-1259.71	-1259.88	703.00	0.63
BHandH	QZVP	-1260.86	-1260.92	-1261.03	-1259.63	-1259.74	-1259.90	704.78	0.37
BHandH	def2SV	-1260.66	-1260.72	-1260.83	-1259.43	-1259.54	-1259.70	710.37	0.42
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		-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		-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	-1261.58	-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		-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	-1261.21	-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	0.07
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	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-pVQZ	-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	-1261.50	-1261.63	707.50	0.21
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	-1262.56	-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	0.17
M06L	TZV	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.43	0.71
M06L	TZVP	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.28	0.73
M06L	QZVP	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	704.95	0.35
M06L	def2SV	-1262.43	-1262.47	-1262.56	-1261.17	-1261.27	-1261.44	708.64	0.17
M06L	def2SVP	-1262.43	-1262.47	-1262.57	-1261.18	-1261.31	-1261.44	709.26	0.26
M06L	def2SVPP	-1262.43	-1262.47	-1262.56	-1261.17	-1261.30	-1261.44	708.64	0.17
M06L	def2TZV	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.43	0.71
M06L	def2TZVP	-1262.59	-1262.64	-1262.73	-1261.36	-1261.45	-1261.61	702.86	0.64
M06L	def2TZVPP	-1262.59	-1262.66	-1262.73	-1261.36	-1261.49	-1261.61	702.96	0.63
M06L	def2QZV	-1262.62	-1262.66	-1262.76	-1261.38	-1261.47	-1261.64	703.80	0.51
M06L	def2QZVP	-1262.62	-1262.67	-1262.76	-1261.38	-1261.47	-1261.64	704.95	0.35
M06L	def2QZVPP	-1262.62	-1262.69	-1262.76	-1261.38	-1261.47	-1261.64	705.02	0.34
SOGGA11		-1248.16	-1248.76	-1248.83	-1247.97	-1248.02	-1248.13	440.87	37.68

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		-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	-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	4.25
M11L	def2QZV	-1262.87	-1262.86	-1262.89	-1261.61	-1261.63	-1261.73	732.53	3.55

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
N12	def2SVPP	-1262.85	-1262.90	-1262.99	-1261.65	-1261.60	-1261.77	760.28	7.47
N12	def2TZV	-1263.03	-1263.10	-1263.16	-1261.84	-1261.84	-1261.97	745.42	5.37

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
VSXC	SVP	-1262.92	-1263.01	-1263.10	-1261.71	-1261.78	-1261.95	718.41	1.55
VSXC	TZV	-1263.09	-1263.18	-1263.26	-1261.93	-1261.96	-1262.13	710.28	0.40
VSXC	TZVP	-1263.09	-1263.18	-1263.26	-1261.93	-1261.96	-1262.13	710.48	0.43
VSXC	QZVP	-1263.12	-1263.21	-1263.30	-1261.97	-1261.99	-1262.16	711.86	0.63
VSXC	def2SV	-1262.92	-1262.98	-1263.10	-1261.75	-1261.74	-1261.95	718.41	1.55

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
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-pVQZ	-1263.27	-1263.36	-1263.44	-1262.09	-1262.15	-1262.28	731.67	3.43
tHCTH	SV	-1263.07	-1263.16	-1263.24	-1261.87	-1261.93	-1262.07	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	-1262.08	-1262.28	730.08	3.20
tHCTH	def2SV	-1263.08	-1263.16	-1263.25	-1261.87	-1261.87	-1262.07	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	4.00
tHCTH	def2TZV	-1263.24	-1263.32	-1263.41	-1262.05	-1262.12	-1262.25	728.92	3.04
tHCTH	def2TZVP	-1263.24	-1263.32	-1263.40	-1262.06	-1262.12	-1262.25	725.23	2.52
tHCTH	def2TZVPP	-1263.24	-1263.33	-1263.41	-1262.06	-1262.12	-1262.25	729.94	3.18
tHCTH	def2QZV	-1263.27	-1263.35	-1263.44	-1262.08	-1262.15	-1262.28	729.44	3.11
tHCTH	def2QZVP	-1263.27	-1263.36	-1263.44	-1262.09	-1262.15	-1262.28	730.08	3.20
tHCTH	def2QZVPP	-1263.27	-1263.35	-1263.44	-1262.09	-1262.15	-1262.28	730.50	3.26
B97D		-1248.83	-1249.44	-1249.59	-1248.50	-1248.57	-1248.71	549.31	22.35
B97D	6-31g	-1262.91	-1263.00	-1263.07	-1261.75	-1261.73	-1261.92	720.79	1.89
B97D	6-31g(d,p)	-1262.91	-1262.99	-1263.07	-1261.75	-1261.73	-1261.92	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
B97D	SVP	-1262.90	-1262.98	-1263.06	-1261.72	-1261.78	-1261.90	731.10	3.35
B97D	TZV	-1263.07	-1263.15	-1263.23	-1261.90	-1261.96	-1262.08	723.45	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
HCTH	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
HCTH	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	728.52	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	-1263.01	-1263.24	-1263.32	-1261.96	-1262.03	-1262.16	730.09	3.20
HCTH	def2QZVPP	-1263.01	-1263.08	-1263.32	-1261.96	-1261.94	-1262.16	730.07	3.20
HCTH93		-1248.80	-1249.62	-1249.59	-1248.66	-1248.63	-1248.88	464.31	34.37
HCTH93	6-31g	-1263.04	-1263.12	-1263.21	-1261.87	-1261.86	-1262.07	720.23	1.81
HCTH93	6-31g(d,p)	-1262.89	-1263.12	-1263.21	-1261.87	-1261.94	-1262.07	720.39	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	2.52
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	-1262.05	-1262.11	-1262.24	725.34	2.53
HCTH93	cc-pVQZ	-1263.23	-1263.31	-1263.40	-1262.05	-1262.12	-1262.24	726.11	2.64
HCTH93	AUG-cc-pVDZ	-1263.22	-1263.31	-1263.39	-1262.04	-1262.02	-1262.24	727.13	2.79
HCTH93	AUG-cc-pVTZ	-1263.22	-1263.31	-1263.40	-1262.05	-1262.03	-1262.24	725.36	2.54
HCTH93	AUG-cc-pVQZ	-1263.23	-1263.32	-1263.40	-1262.05	-1262.12	-1262.24	726.11	2.64

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		-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	-1263.05	-1263.13	-1261.78	-1261.84	-1261.97	727.04	2.77
HCTH147	cc-pVDZ	-1263.07	-1263.21	-1263.30	-1261.94	-1261.92	-1262.13	729.65	3.14
HCTH147	cc-pVTZ	-1263.08	-1263.22	-1263.30	-1261.88	-1262.01	-1262.14	728.31	2.95
HCTH147	cc-pVQZ	-1262.97	-1263.15	-1263.31	-1261.95	-1262.02	-1262.14	728.97	3.05
HCTH147	AUG-cc-pVDZ	-1262.96	-1263.22	-1263.30	-1261.94	-1261.94	-1262.14	729.61	3.14
HCTH147	AUG-cc-pVTZ	-1263.13	-1263.21	-1263.30	-1261.95	-1262.01	-1262.14	728.32	2.95
HCTH147	AUG-cc-pVQZ	-1262.98	-1263.22	-1263.31	-1261.88	-1262.02	-1262.14	728.97	3.05
HCTH147	SV	-1262.75	-1262.96	-1263.11	-1261.73	-1261.80	-1261.93	738.18	4.35
HCTH147	SVP	-1262.75	-1262.96	-1263.10	-1261.74	-1261.80	-1261.94	733.77	3.73
HCTH147	TZV	-1262.95	-1263.08	-1263.27	-1261.83	-1261.98	-1262.11	726.48	2.69
HCTH147	TZVP	-1262.92	-1263.18	-1263.27	-1261.83	-1261.98	-1262.11	726.71	2.73
HCTH147	QZVP	-1263.13	-1263.21	-1263.30	-1261.95	-1262.01	-1262.14	728.52	2.98
HCTH147	def2SV	-1262.93	-1263.02	-1263.11	-1261.74	-1261.73	-1261.94	734.90	3.89
HCTH147	def2SVP	-1262.93	-1263.03	-1263.10	-1261.74	-1261.80	-1261.94	733.77	3.72
HCTH147	def2SVPP	-1262.93	-1263.02	-1263.11	-1261.74	-1261.80	-1261.94	734.90	3.89
HCTH147	def2TZV	-1262.95	-1263.18	-1263.27	-1261.92	-1261.98	-1262.11	726.49	2.70
HCTH147	def2TZVP	-1262.94	-1263.19	-1263.27	-1261.92	-1261.98	-1262.12	727.12	2.78
HCTH147	def2TZVPP	-1262.92	-1263.12	-1263.28	-1261.92	-1261.99	-1262.12	727.89	2.89
HCTH147	def2QZV	-1263.08	-1263.15	-1263.30	-1261.95	-1262.01	-1262.14	727.41	2.83
HCTH147	def2QZVP	-1263.08	-1263.10	-1263.30	-1261.95	-1262.01	-1262.14	728.52	2.98
HCTH147	def2QZVPP	-1263.13	-1263.22	-1263.30	-1261.95	-1261.93	-1262.14	728.73	3.01
HCTH407		-1249.18	-1249.52	-1249.68	-1248.56	-1248.53	-1248.79	558.47	21.06
HCTH407	6-31g	-1262.79	-1263.05	-1263.14	-1261.71	-1261.85	-1261.98	726.57	2.71
HCTH407	6-31g(d,p)	-1262.85	-1263.05	-1263.14	-1261.70	-1261.85	-1261.98	726.60	2.71
HCTH407	6-31+g	-1262.83	-1263.06	-1263.15	-1261.79	-1261.86	-1261.98	730.59	3.27
HCTH407	6-31+g(d,p)	-1262.98	-1263.07	-1263.15	-1261.79	-1261.80	-1261.98	732.70	3.57
HCTH407	6-31++g	-1262.83	-1263.06	-1263.15	-1261.79	-1261.86	-1261.98	732.36	3.52
HCTH407	6-31++g(d,p)	-1262.83	-1263.07	-1263.15	-1261.79	-1261.80	-1261.98	730.83	3.31
HCTH407	cc-pVDZ	-1263.05	-1263.23	-1263.32	-1261.95	-1262.02	-1262.15	732.17	3.50
HCTH407	cc-pVTZ	-1263.14	-1263.11	-1263.32	-1261.96	-1262.03	-1262.16	729.80	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	-1263.04	-1263.13	-1261.75	-1261.74	-1261.95	737.31	4.23
HCTH407	def2SVP	-1262.82	-1263.04	-1263.13	-1261.75	-1261.82	-1261.95	738.17	4.35
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	-1261.93	-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	-1263.21	-1263.29	-1261.94	-1262.00	-1262.13	729.23	3.08
HCTH407	def2QZV	-1263.10	-1263.13	-1263.32	-1261.88	-1262.03	-1262.16	730.02	3.19
HCTH407	def2QZVP	-1263.01	-1263.11	-1263.32	-1261.96	-1262.03	-1262.16	730.09	3.20
HCTH407	def2QZVPP	-1263.00	-1263.18	-1263.32	-1261.96	-1262.03	-1262.16	730.07	3.20
B2PLYP		-1248.45	-1248.73	-1248.97	-1247.81	-1247.84	-1248.08	555.88	21.42
B2PLYP	6-31g	-1262.16	-1262.22	-1262.32	-1260.95	-1261.05	-1261.21	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	-1262.23	-1262.34	-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	701.77	0.80
B2PLYP	6-31++g	-1262.18	-1262.23	-1262.34	-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	701.77	0.80
B2PLYP	cc-pVDZ	-1262.34	-1262.36	-1262.50	-1261.12	-1261.22	-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	-1261.38	700.68	0.95
B2PLYP	AUG-cc-pVQZ	-1262.34	-1262.36	-1262.50	-1261.13	-1261.23	-1261.39	701.02	0.90
B2PLYP	SV	-1262.15	-1262.20	-1262.31	-1260.92	-1261.02	-1261.18	708.99	0.22
B2PLYP	SVP	-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		-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 Kcal/mol	%Error
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

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
PBE0DH	6-31+g(d,p)	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	706.01	0.20
PBE0DH	6-31++g	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	705.49	0.27
PBE0DH	6-31++g(d,p)	-1262.17	-1262.23	-1262.34	-1260.94	-1261.05	-1261.21	706.01	0.20
PBE0DH	cc-pVDZ	-1262.33	-1262.35	-1262.50	-1261.10	-1261.17	-1261.37	707.87	0.06
PBE0DH	cc-pVTZ	-1262.33	-1262.39	-1262.50	-1261.11	-1261.21	-1261.38	704.92	0.35
PBE0DH	cc-pVQZ	-1262.33	-1262.39	-1262.50	-1261.11	-1261.22	-1261.38	705.34	0.29
PBE0DH	AUG-cc-pVDZ	-1262.33	-1262.35	-1262.50	-1261.10	-1261.21	-1261.37	707.71	0.04
PBE0DH	AUG-cc-pVTZ	-1262.33	-1262.36	-1262.50	-1261.11	-1261.22	-1261.38	704.94	0.35
PBE0DH	AUG-cc-pVQZ	-1262.33	-1262.36	-1262.50	-1261.11	-1261.22	-1261.38	705.33	0.29
PBE0DH	SV	-1262.14	-1262.20	-1262.31	-1260.90	-1261.01	-1261.17	713.54	0.87
PBE0DH	SVP	-1262.14	-1262.20	-1262.31	-1260.91	-1260.97	-1261.18	711.01	0.51
PBE0DH	TZV	-1262.30	-1262.36	-1262.47	-1261.08	-1261.19	-1261.35	703.28	0.59
PBE0DH	TZVP	-1262.30	-1262.36	-1262.47	-1261.08	-1261.19	-1261.35	703.33	0.58
PBE0DH	QZVP	-1262.33	-1262.39	-1262.50	-1261.11	-1261.22	-1261.38	705.20	0.31
PBE0DH	def2SV	-1262.14	-1262.20	-1262.31	-1260.91	-1261.01	-1261.18	711.01	0.51
PBE0DH	def2SVP	-1262.14	-1262.20	-1262.31	-1260.91	-1261.01	-1261.18	712.00	0.65
PBE0DH	def2SVPP	-1262.14	-1262.20	-1262.31	-1260.91	-1261.01	-1261.18	711.01	0.51
PBE0DH	def2TZV	-1262.30	-1262.36	-1262.47	-1261.08	-1261.19	-1261.35	703.28	0.59
PBE0DH	def2TZVP	-1262.30	-1262.36	-1262.48	-1261.08	-1261.19	-1261.35	704.12	0.47
PBE0DH	def2TZVPP	-1262.31	-1262.37	-1262.48	-1261.09	-1261.19	-1261.35	704.63	0.39
PBE0DH	def2QZV	-1262.33	-1262.39	-1262.50	-1261.11	-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		-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	-1262.14	-1262.16	-1262.31	-1260.93	-1261.04	-1261.21	693.95	1.90
PBEQIDH	AUG-cc-pVTZ	-1262.14	-1262.20	-1262.32	-1260.94	-1261.01	-1261.22	690.77	2.35
PBEQIDH	AUG-cc-pVQZ	-1262.14	-1262.20	-1262.32	-1260.94	-1261.05	-1261.22	691.15	2.30
PBEQIDH	SV	-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	-1262.29	-1260.90	-1261.02	-1261.19	688.92	2.62
PBEQIDH	QZVP	-1262.14	-1262.20	-1262.32	-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	-1261.02	697.55	1.39
PBEQIDH	def2SVPP	-1261.95	-1262.01	-1262.13	-1260.73	-1260.84	-1261.02	696.29	1.57
PBEQIDH	def2TZV	-1262.11	-1262.17	-1262.29	-1260.90	-1261.02	-1261.19	688.92	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	688.93	2.61
PBEQIDH	def2QZVP	-1262.14	-1262.20	-1262.32	-1260.94	-1261.04	-1261.22	691.01	2.32
PBEQIDH	def2QZVPP	-1262.14	-1262.20	-1262.32	-1260.94	-1261.04	-1261.22	691.10	2.31
MP2		-1247.69	-1247.77	-1248.07	-1246.88	-1247.28	-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		-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	-1261.57	-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	-1262.99	-1263.07	-1261.73	-1261.70	-1261.91	725.26	2.52
OPBE	cc-pVTZ	-1262.67	-1262.99	-1263.07	-1261.74	-1261.80	-1261.92	722.98	2.20
OPBE	cc-pVQZ	-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	-1261.91	725.16	2.51
OPBE	AUG-cc-pVTZ	-1262.83	-1262.99	-1263.07	-1261.74	-1261.80	-1261.92	723.02	2.21
OPBE	AUG-cc-pVQZ	-1262.73	-1262.98	-1263.07	-1261.75	-1261.80	-1261.92	723.56	2.28
OPBE	SV	-1262.52	-1262.79	-1262.87	-1261.53	-1261.58	-1261.71	732.85	3.59
OPBE	SVP	-1262.64	-1262.79	-1262.88	-1261.53	-1261.59	-1261.71	730.15	3.21
OPBE	TZV	-1262.68	-1262.96	-1263.04	-1261.71	-1261.77	-1261.89	721.65	2.01
OPBE	TZVP	-1262.71	-1262.96	-1263.04	-1261.71	-1261.77	-1261.89	721.78	2.03
OPBE	QZVP	-1262.84	-1262.98	-1263.07	-1261.74	-1261.80	-1261.92	723.22	2.23
OPBE	def2SV	-1262.64	-1262.79	-1262.88	-1261.53	-1261.51	-1261.71	730.15	3.21
OPBE	def2SVP	-1262.51	-1262.80	-1262.88	-1261.53	-1261.59	-1261.71	730.70	3.29
OPBE	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