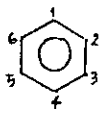
LAMPIRAN I

HASIL PERHITUNGAN UNTUK MOLEKUL BENZENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk benzena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)
-2.000	0.408	0.408	0.408	0.408	0.408	0.408
-1.000	0.577	0.285	-0.292	-0.577	-0.285	0.292
-1.000	0.004	0.502	0.498	-0.004	-0.502	-0.498
1.000	0.575	-0.243	-0.332	0.575	-0.243	-0.332
1.000	0.051	-0.524	0.472	0.051	-0.524	0.472
2.000	0.408	-0.408	0.408	-0.408	0.408	-0.408

Energi elektron π (sebelum tehnik w) untuk benzena

E = 6.0000 α +8.0000 β

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)
1.000	1.000	1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
-0.000	0.000	-0.000	-0.000	0.000	-0.000

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 6)	(2 3)	(3 4)	(4 5)	(5 6)
0.667	0.667	0.667	0.667	0.667	0.667

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)
0.399	0.399	0.399	0.399	0.399	0.399

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Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)
0.00	0.50	0.50	0.00	0.50	0.50

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)
0.66	0.12	0.22	0.66	0.12	0.22

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)
0.33	0.31	0.36	0.33	0.31	0.36

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)
0.83	0.83	0.83	0.83	0.83	0.83

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)
0.83	0.83	0.83	0.83	0.83	0.83

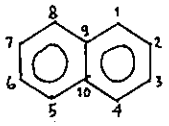
Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)
0.83	0.83	0.83	0.83	0.83	0.83

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LAMPIRAN II

HASIL PERHITUNGAN UNTUK MOLEKUL NAFTALENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk naftalena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.303	0.301	0.231	0.231	0.301	0.301	0.231	0.231
-1.618	0.263	0.425	0.425	0.263	-0.263	-0.425	-0.425
-1.303	0.400	0.174	-0.174	-0.400	-0.400	-0.174	0.174
-1.000	0.000	0.408	0.408	0.000	-0.000	0.408	0.408
-0.618	0.425	0.263	-0.263	-0.425	0.425	0.263	-0.263
0.618	0.425	-0.263	-0.263	0.425	-0.425	0.263	0.263
1.000	0.000	0.408	-0.408	0.000	0.000	-0.408	0.408
1.303	0.400	-0.173	-0.174	0.400	0.400	-0.173	-0.174
1.618	0.263	-0.425	0.425	-0.263	0.263	-0.425	0.425
2.303	0.301	-0.231	0.231	-0.301	-0.301	0.231	-0.231

X	C(8)	C(9)	C(10)
-2.303	0.301	0.461	0.461
-1.618	-0.263	0.000	0.000
-1.303	0.400	0.347	-0.347
-1.000	-0.000	-0.408	-0.408
-0.618	-0.425	-0.000	0.000
0.618	-0.425	-0.000	-0.000
1.000	0.000	-0.408	0.408
1.303	0.400	-0.347	-0.347
1.618	-0.263	-0.000	-0.000
2.303	0.301	-0.461	0.461

Energi elektron π (sebelum tehnik w) untuk naftalena

$E = 10.0000\ \alpha + 13.6832\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)
1.000	1.000	1.000

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Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	0.000	-0.000	-0.000	-0.000	0.000	0.000

f(8)	f(9)	f(10)
-0.000	-0.000	0.000

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 9)	(2 3)	(3 4)	(4 10)	(5 6)	(5 10)
0.725	0.555	0.603	0.725	0.555	0.725	0.555

(6 7)	(7 8)	(8 9)	(9 10)
0.603	0.725	0.555	0.518

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.453	0.404	0.404	0.453	0.453	0.404	0.404

Fv(8)	Fv(9)	Fv(10)
0.453	0.104	0.104

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.36	0.14	0.14	0.36	0.36	0.14	0.14

fe(8)	fe(9)	fe(10)
0.36	0.00	0.00

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.36	0.14	0.14	0.36	0.36	0.14	0.14

fn(8)	fn(9)	fn(10)
0.36	0.00	0.00

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.36	0.14	0.14	0.36	0.36	0.14	0.14

fr(8)	fr(9)	fr(10)
0.36	0.00	0.00

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.99	0.87	0.87	0.99	0.99	0.87	0.87

Se(8)	Se(9)	Se(10)
0.99	0.70	0.70

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.99	0.87	0.87	0.99	0.99	0.87	0.87

Sn(8)	Sn(9)	Sn(10)
0.99	0.70	0.70

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

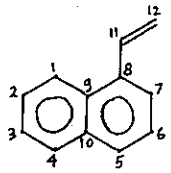
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.99	0.87	0.87	0.99	0.99	0.87	0.87

Sr(8)	Sr(9)	Sr(10)
0.99	0.70	0.70

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LAMPIRAN III

HASIL PERHITUNGAN UNTUK MOLEKUL 1-VINILNAFTALENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk 1-vinilnaftalena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.365	0.279	0.200	0.194	0.259	0.272	0.225	0.259
-1.732	0.204	0.354	0.408	0.354	0.000	-0.204	-0.354
-1.469	0.327	0.304	0.120	-0.128	-0.501	-0.428	-0.128
-1.000	0.433	0.147	-0.286	-0.433	0.000	0.147	0.147
-1.000	0.003	-0.407	-0.410	-0.003	0.000	-0.407	-0.407
-0.498	0.293	0.234	-0.177	-0.322	0.418	0.193	-0.322
0.498	0.293	-0.234	-0.177	0.322	-0.418	0.193	0.322
1.000	0.021	-0.415	0.394	0.021	0.000	0.415	-0.415
1.000	0.433	-0.124	-0.308	0.433	0.000	0.124	-0.124
1.469	0.327	-0.304	0.120	0.128	0.501	-0.428	0.128
1.732	0.204	-0.353	0.408	-0.354	0.000	-0.204	0.354
2.365	0.279	-0.200	0.194	-0.259	-0.272	0.225	-0.259

X	C(8)	C(9)	C(10)	C(11)	C(12)
-2.365	0.389	0.460	0.419	0.200	0.085
-1.732	-0.408	0.000	0.204	-0.354	-0.204
-1.469	0.240	0.176	-0.308	0.304	0.207
-1.000	0.000	0.286	-0.147	-0.433	-0.433
-1.000	0.000	0.410	0.407	-0.003	-0.003
-0.498	-0.353	-0.088	0.016	0.234	0.470
0.498	-0.353	0.088	0.016	-0.234	0.470
1.000	0.000	0.394	-0.415	0.021	-0.021
1.000	0.000	-0.308	-0.124	0.432	-0.432
1.469	0.240	-0.176	-0.308	-0.304	0.207
1.732	-0.408	0.000	0.204	0.354	-0.204
2.365	0.389	-0.460	0.419	-0.200	0.085

Energi elektron π (sebelum tehnik w) untuk 1-vinilnaftalena

$E = 12.0000\ \alpha + 16.1294\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

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q(8)	q(9)	q(10)	q(11)	q(12)
1.000	1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	0.000	0.000	0.000	-0.000	-0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)
0.000	0.000	-0.000	0.000	-0.000

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 9)	(2 3)	(3 4)	(4 10)	(5 6)	(5 10)
0.717	0.570	0.607	0.723	0.555	0.712	0.550

(6 7)	(7 8)	(8 9)	(8 11)	(9 10)	(11 12)
0.621	0.656	0.504	0.425	0.524	0.899

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.444	0.408	0.403	0.454	0.469	0.398	0.454

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)
0.147	0.134	0.103	0.408	0.833

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.17	0.11	0.06	0.21	0.35	0.07	0.21

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)
0.25	0.02	0.00	0.11	0.44

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.17	0.11	0.06	0.21	0.35	0.07	0.21

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)
0.25	0.02	0.00	0.11	0.44

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.17	0.11	0.06	0.21	0.35	0.07	0.21

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)
0.25	0.02	0.00	0.11	0.44

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.98	0.90	0.87	1.02	1.11	0.86	1.02

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)
0.90	0.75	0.70	0.90	1.37

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.98	0.90	0.87	1.02	1.11	0.86	1.02

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)
0.90	0.75	0.70	0.90	1.37

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

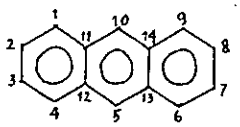
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.98	0.90	0.87	1.02	1.11	0.86	1.02

Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)
0.90	0.75	0.70	0.90	1.37

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LAMPIRAN IV

HASIL PERHITUNGAN UNTUK MOLEKUL ANTRASENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk antrasena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.414	0.215	0.152	0.152	0.215	0.304	0.215	0.152
-2.000	0.289	0.289	0.289	0.289	-0.000	-0.289	-0.289
-1.414	0.168	0.406	0.406	0.169	-0.237	0.169	0.406
-1.414	0.281	0.117	-0.116	-0.281	-0.398	-0.280	-0.115
-1.000	0.408	0.203	-0.205	-0.408	0.000	0.408	0.205
-1.000	0.001	0.354	0.353	-0.001	0.000	0.001	-0.353
-0.414	0.311	0.220	-0.220	-0.311	0.440	-0.311	-0.220
0.414	0.311	-0.220	-0.220	0.311	-0.440	0.311	-0.220
1.000	0.002	0.353	-0.355	0.002	0.000	-0.002	0.354
1.000	0.408	-0.206	-0.202	0.408	0.000	-0.408	0.202
1.414	0.291	-0.142	-0.090	0.269	0.412	0.269	-0.090
1.414	0.150	-0.398	0.413	-0.186	0.212	-0.186	0.413
2.000	0.289	-0.289	0.289	-0.289	-0.000	0.289	-0.289
2.414	0.215	-0.152	0.152	-0.215	-0.304	-0.215	0.152

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.414	0.152	0.215	0.304	0.367	0.367	0.367	0.367
-2.000	-0.289	-0.289	-0.000	0.289	0.289	-0.289	-0.289
-1.414	0.406	0.168	-0.239	-0.169	-0.168	-0.168	-0.169
-1.414	0.117	0.281	0.397	0.280	-0.281	-0.281	0.280
-1.000	-0.203	-0.408	-0.000	0.205	-0.203	0.203	-0.205
-1.000	-0.354	-0.001	-0.000	-0.353	-0.354	0.354	0.353
-0.414	0.220	0.311	-0.440	-0.091	0.091	0.091	-0.091
0.414	-0.220	0.311	-0.440	0.091	0.091	0.091	0.091
1.000	-0.353	-0.002	0.000	-0.355	0.353	-0.353	0.354
1.000	0.206	-0.408	0.000	-0.203	-0.206	0.206	0.202
1.414	-0.142	0.291	0.381	-0.269	-0.291	-0.291	-0.269
1.414	-0.398	0.150	-0.263	0.186	-0.150	-0.150	0.186
2.000	0.289	-0.289	-0.000	-0.289	0.289	-0.289	0.289
2.414	-0.152	0.215	0.304	-0.367	0.367	0.367	-0.367

Energi elektron π (sebelum tehnik w) untuk antrasena

$E = 14.0000\ \alpha + 19.3137\ \beta$

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Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	0.000	0.000	-0.000	0.000	-0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.000	0.000	-0.000	0.000	-0.000	0.000	-0.000

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 11)	(2 3)	(3 4)	(4 12)	(5 12)	(5 13)
0.737	0.535	0.586	0.737	0.535	0.606	0.606

(6 7)	(6 13)	(7 8)	(8 9)	(9 14)	(10 11)	(10 14)
0.737	0.535	0.586	0.737	0.535	0.606	0.606

(11 12)	(13 14)
0.485	0.485

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.459	0.409	0.409	0.459	0.520	0.459	0.409

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.409	0.459	0.520	0.106	0.106	0.106	0.106

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.19	0.10	0.10	0.19	0.39	0.19	0.10

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.10	0.19	0.39	0.02	0.02	0.02	0.02

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Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.19	0.10	0.10	0.19	0.39	0.19	0.10

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.10	0.19	0.39	0.02	0.02	0.02	0.02

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.19	0.10	0.10	0.19	0.39	0.19	0.10

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.10	0.19	0.39	0.02	0.02	0.02	0.02

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
1.07	0.92	0.92	1.07	1.31	1.07	0.92

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.92	1.07	1.31	0.72	0.72	0.72	0.72

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.07	0.92	0.92	1.07	1.31	1.07	0.92

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.92	1.07	1.31	0.72	0.72	0.72	0.72

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

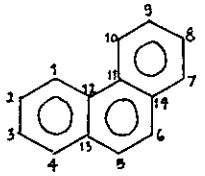
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.07	0.92	0.92	1.07	1.31	1.07	0.92

Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.92	1.07	1.31	0.72	0.72	0.72	0.72

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LAMPIRAN V

HASIL PERHITUNGAN UNTUK MOLEKUL FENANTRENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk fenantrena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.435	0.233	0.157	0.150	0.207	0.248	0.248	0.207
-1.951	0.246	0.287	0.314	0.326	0.109	-0.109	-0.326
-1.516	0.292	0.325	0.202	-0.019	-0.448	-0.448	-0.019
-1.306	0.149	-0.197	-0.406	-0.333	-0.097	-0.097	-0.333
-1.142	0.297	0.386	0.144	-0.221	-0.185	0.185	0.221
-0.769	0.369	-0.026	-0.389	-0.273	0.101	-0.101	0.273
-0.605	0.233	0.315	-0.042	-0.340	0.415	0.415	-0.340
0.605	0.233	-0.315	-0.042	0.340	-0.415	0.415	-0.340
0.769	0.369	0.026	-0.389	0.273	-0.101	-0.101	0.273
1.142	0.297	-0.386	0.144	0.221	0.185	0.185	0.221
1.306	0.149	0.197	-0.406	0.333	0.096	-0.097	-0.333
1.516	0.292	-0.325	0.202	0.020	0.448	-0.448	-0.020
1.951	0.246	-0.287	0.314	-0.326	-0.109	-0.109	-0.326
2.435	0.233	-0.157	0.150	-0.207	-0.248	0.248	0.207

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.435	0.150	0.157	0.233	0.410	0.410	0.355	0.355
-1.951	-0.314	-0.287	-0.246	-0.192	0.192	0.321	-0.321
-1.516	0.202	0.325	0.292	0.117	0.117	-0.231	-0.231
-1.306	-0.406	-0.197	0.149	0.391	0.391	-0.030	-0.030
-1.142	-0.144	-0.386	-0.297	0.047	-0.047	-0.397	0.397
-0.769	0.389	0.026	-0.369	-0.309	0.309	0.179	-0.179
-0.605	-0.042	0.315	0.233	-0.174	-0.174	-0.164	-0.164
0.605	0.042	0.315	-0.233	-0.174	0.174	-0.164	0.164
0.769	-0.389	0.026	0.369	-0.309	-0.309	0.179	0.179
1.142	0.144	-0.386	0.297	0.047	0.047	-0.397	-0.397
1.306	0.406	-0.197	-0.149	0.391	-0.391	-0.030	0.030
1.516	-0.202	0.325	-0.292	0.117	-0.117	-0.231	0.231
1.951	0.314	-0.287	0.246	-0.192	-0.192	0.321	0.322
2.435	-0.150	0.157	-0.233	0.410	-0.410	0.355	-0.355

Energi elektron π (sebelum tehnik w) untuk fenantrena

$E = 14.0000\ \alpha + 19.4483\ \beta$

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Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	-0.000	0.000	-0.000	0.000	0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.000	0.000	0.000	-0.000	0.000	-0.000	-0.000

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 12)	(2 3)	(3 4)	(4 13)	(5 6)	(5 13)
0.702	0.590	0.623	0.707	0.575	0.775	0.506

(6 14)	(7 8)	(7 14)	(8 9)	(9 10)	(10 11)	(11 12)
0.506	0.707	0.575	0.623	0.702	0.590	0.461

(11 14)	(12 13)
0.542	0.542

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.440	0.408	0.402	0.450	0.451	0.451	0.450

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.402	0.408	0.440	0.139	0.139	0.109	0.109

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.11	0.20	0.00	0.23	0.34	0.34	0.23

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.00	0.20	0.11	0.06	0.06	0.05	0.05

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Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.11	0.20	0.00	0.23	0.34	0.34	0.23

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.00	0.20	0.11	0.06	0.06	0.05	0.05

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.11	0.20	0.00	0.23	0.34	0.34	0.23

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.00	0.20	0.11	0.06	0.06	0.05	0.05

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.94	0.89	0.86	0.98	1.00	1.00	0.98

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.86	0.89	0.94	0.78	0.78	0.73	0.73

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.94	0.89	0.86	0.98	1.00	1.00	0.98

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.86	0.89	0.94	0.78	0.78	0.73	0.73

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

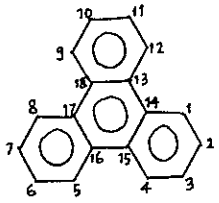
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.94	0.89	0.86	0.98	1.00	1.00	0.98

Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.86	0.89	0.94	0.78	0.78	0.73	0.73

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LAMPIRAN VI

HASIL PERHITUNGAN UNTUK MOLEKUL TRIFENILENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk trifenilena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.532	0.183	0.120	0.120	0.183	0.183	0.120	0.120
-1.970	0.075	0.017	-0.041	-0.097	-0.319	-0.297	-0.266
-1.970	0.325	0.333	0.331	0.319	-0.097	-0.151	-0.200
-1.347	0.120	0.345	0.345	0.120	0.120	0.345	0.345
-1.286	0.323	0.144	-0.138	-0.321	-0.089	0.188	0.332
-1.286	0.083	0.301	0.303	0.089	-0.321	-0.275	-0.032
-0.879	0.345	0.183	-0.183	-0.345	0.345	0.183	-0.183
-0.684	0.330	0.156	-0.223	-0.309	-0.125	-0.333	-0.102
-0.684	0.046	-0.295	-0.247	0.125	-0.309	0.012	0.317
0.684	0.105	0.261	-0.284	-0.067	-0.326	0.049	0.293
0.684	0.316	-0.207	-0.174	0.326	-0.067	0.330	-0.159
0.879	0.345	-0.183	-0.183	0.345	0.345	-0.183	-0.183
1.286	0.170	-0.329	0.253	0.003	-0.333	0.212	0.061
1.286	0.287	-0.055	-0.217	0.333	0.003	-0.257	0.328
1.347	0.120	-0.344	0.345	-0.120	0.120	-0.345	0.345
1.970	0.322	-0.301	0.272	-0.235	-0.237	0.274	-0.303
1.970	0.088	-0.142	0.193	-0.237	0.235	-0.190	0.139
2.532	0.183	-0.120	0.120	-0.183	0.183	-0.120	0.120

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.532	0.183	0.183	0.120	0.120	0.183	0.345	0.345
-1.970	-0.227	0.244	0.280	0.307	0.325	0.333	0.130
-1.970	-0.244	-0.227	-0.182	-0.130	-0.075	-0.017	0.307
-1.347	0.120	0.120	0.344	0.344	0.120	-0.183	-0.183
-1.286	0.238	-0.233	-0.332	-0.194	0.083	0.301	0.271
-1.286	0.233	0.238	-0.026	-0.271	-0.323	-0.144	-0.194
-0.879	-0.345	0.345	0.183	-0.183	-0.345	-0.120	0.120
-0.684	0.263	-0.205	0.177	0.326	0.046	-0.295	0.070
-0.684	0.205	0.263	0.282	-0.070	-0.330	-0.156	0.326
0.684	-0.249	0.221	-0.310	-0.009	0.316	-0.207	-0.333
0.684	-0.221	-0.249	-0.123	0.333	-0.105	-0.261	-0.009
0.879	0.345	0.344	-0.183	-0.183	0.344	-0.120	-0.120
1.286	-0.290	0.164	0.117	-0.314	0.287	-0.055	0.111
1.286	-0.164	-0.290	0.312	-0.111	-0.169	0.329	-0.314
1.347	-0.120	0.120	-0.345	0.345	-0.120	-0.183	0.183
1.970	0.322	-0.085	0.027	0.031	-0.088	0.142	-0.332
1.970	-0.085	-0.322	0.332	-0.332	0.322	-0.301	-0.031
2.532	-0.183	0.183	-0.120	0.120	-0.183	0.345	-0.345

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X	C(15)	C(16)	C(17)	C(18)
-2.532	0.345	0.345	0.345	0.345
-1.970	-0.151	-0.331	-0.182	0.201
-1.970	0.297	-0.041	-0.280	-0.266
-1.347	-0.184	-0.184	-0.183	-0.183
-1.286	-0.275	-0.303	-0.026	0.032
-1.286	-0.188	-0.138	0.332	0.332
-0.879	-0.120	0.120	-0.120	0.120
-0.684	0.012	0.247	0.282	-0.317
-0.684	0.333	-0.223	-0.177	-0.102
0.684	0.330	0.175	-0.123	0.159
0.684	-0.049	-0.284	0.310	0.293
0.879	-0.120	-0.120	-0.120	-0.120
1.286	-0.257	0.217	0.312	-0.328
1.286	-0.212	0.253	-0.117	0.061
1.347	-0.183	0.183	-0.183	0.183
1.970	0.190	0.193	-0.332	0.139
1.970	0.274	-0.272	0.027	0.303
2.532	0.345	-0.345	0.345	-0.345

Energi elektron π (sebelum tehnik w)
untuk trifenilena

$E = 18.0000\ \alpha + 25.2745\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)	q(17)	q(18)
1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	0.000	0.000	-0.000	-0.000	-0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.000	0.000	0.000	-0.000	0.000	-0.000	-0.000

f(15)	f(16)	f(17)	f(18)
0.000	0.000	0.000	-0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 14)	(2 3)	(3 4)	(4 15)	(5 6)	(5 16)
0.690	0.603	0.637	0.690	0.603	0.690	0.603

(6 7)	(7 8)	(8 17)	(9 10)	(9 18)	(10 11)	(11 12)
0.637	0.690	0.603	0.690	0.603	0.637	0.690

(12 13)	(13 14)	(13 18)	(14 15)	(15 16)	(16 17)	(17 18)
0.603	0.428	0.562	0.562	0.428	0.562	0.428

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.439	0.405	0.405	0.439	0.439	0.405	0.405

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.439	0.439	0.405	0.405	0.439	0.140	0.140

Fv(15)	Fv(16)	Fv(17)	Fv(18)
0.140	0.140	0.140	0.140

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.00	0.17	0.12	0.03	0.19	0.00	0.20

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.08	0.14	0.16	0.01	0.22	0.05	0.21

fe(15)	fe(16)	fe(17)	fe(18)
0.22	0.10	0.06	0.02

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.02	0.14	0.16	0.01	0.21	0.00	0.17

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.12	0.10	0.19	0.00	0.20	0.09	0.22

fn(15)	fn(16)	fn(17)	fn(18)
0.22	0.06	0.03	0.05

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.01	0.15	0.14	0.02	0.20	0.00	0.19

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.10	0.12	0.18	0.00	0.21	0.07	0.22

fr(15)	fr(16)	fr(17)	fr(18)
0.22	0.08	0.05	0.04

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.93	0.87	0.87	0.93	0.93	0.87	0.87

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.93	0.93	0.87	0.87	0.93	0.79	0.79

Se(15)	Se(16)	Se(17)	Se(18)
0.79	0.79	0.79	0.79

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.93	0.87	0.87	0.93	0.93	0.87	0.87

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.93	0.93	0.87	0.87	0.93	0.79	0.79

Sn(15)	Sn(16)	Sn(17)	Sn(18)
0.79	0.79	0.79	0.79

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.93	0.87	0.87	0.93	0.93	0.87	0.87

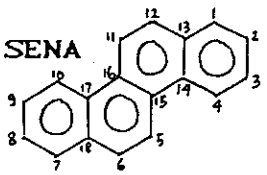
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.93	0.93	0.87	0.87	0.93	0.79	0.79

Sr(15)	Sr(16)	Sr(17)	Sr(18)
0.79	0.79	0.79	0.79

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LAMPIRAN VII

HASIL PERHITUNGAN UNTUK MOLEKUL KRISENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk krisena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.499	0.153	0.107	0.114	0.178	0.231	0.202	0.153
-2.167	0.267	0.223	0.217	0.247	-0.046	-0.185	-0.267
-1.701	0.283	0.348	0.309	0.178	-0.219	-0.051	0.283
-1.540	0.083	-0.071	-0.193	-0.226	-0.384	-0.379	-0.083
-1.286	0.241	-0.010	-0.253	-0.316	0.095	0.323	0.241
-1.216	0.172	0.402	0.317	-0.017	-0.108	0.069	-0.172
-0.875	0.368	0.149	-0.238	-0.357	0.297	0.142	-0.368
-0.792	0.090	0.337	0.178	-0.197	0.292	0.033	0.090
-0.520	0.295	0.120	-0.233	-0.241	-0.234	-0.386	0.295
0.520	0.295	-0.120	-0.233	0.241	-0.234	0.386	-0.296
0.792	0.090	-0.337	0.178	0.197	0.292	-0.033	-0.090
0.875	0.368	-0.149	-0.238	0.357	0.297	-0.142	0.368
1.216	0.172	-0.402	0.317	0.017	-0.108	-0.069	0.172
1.286	0.240	0.010	-0.253	0.316	0.096	-0.323	-0.240
1.540	0.083	0.071	-0.193	0.226	-0.384	0.379	0.083
1.701	0.283	-0.348	0.309	-0.178	-0.219	0.051	-0.283
2.167	0.267	-0.223	0.217	-0.247	-0.046	0.185	0.267
2.499	0.153	-0.107	0.114	-0.178	0.231	-0.202	-0.153

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.499	0.107	0.114	0.178	0.231	0.202	0.275	0.331
-2.167	-0.223	-0.217	-0.247	0.046	0.185	0.355	0.317
-1.701	0.348	0.309	0.178	-0.219	-0.051	0.132	-0.006
-1.540	0.071	0.193	0.226	0.384	0.379	0.200	-0.155
-1.286	-0.010	-0.253	-0.316	0.096	0.322	0.319	-0.153
-1.216	-0.402	-0.317	0.017	0.108	-0.069	-0.193	-0.337
-0.875	-0.149	0.238	0.357	-0.297	-0.142	0.173	-0.075
-0.792	0.337	0.177	-0.197	0.292	0.033	-0.266	-0.333
-0.520	0.120	-0.233	-0.241	-0.234	-0.386	0.033	0.107
0.520	0.120	0.233	-0.241	0.234	-0.385	-0.034	0.107
0.792	0.337	-0.177	-0.197	-0.292	0.033	0.266	-0.333
0.875	-0.149	-0.238	0.357	0.297	-0.142	-0.173	-0.075
1.216	-0.402	0.317	0.017	-0.108	-0.069	0.193	-0.337
1.286	-0.010	0.253	-0.316	-0.096	0.323	-0.319	-0.153
1.540	0.071	-0.193	0.226	-0.384	0.379	-0.200	-0.155
1.701	0.348	-0.309	0.178	0.219	-0.051	-0.133	-0.006
2.167	-0.223	0.217	-0.247	-0.046	0.185	-0.355	0.317
2.499	0.107	-0.114	0.178	-0.231	0.202	-0.275	0.331

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X	C(15)	C(16)	C(17)	C(18)
-2.499	0.375	0.375	0.331	0.275
-2.167	0.086	-0.086	-0.317	-0.355
-1.701	-0.321	-0.321	-0.006	0.132
-1.540	-0.212	0.212	0.155	-0.200
-1.286	-0.200	-0.200	-0.153	0.319
-1.216	-0.201	0.201	0.337	0.193
-0.875	0.118	-0.118	0.075	-0.173
-0.792	0.199	0.199	-0.333	-0.266
-0.520	0.264	0.264	0.107	0.033
0.520	-0.264	0.264	-0.107	0.034
0.792	-0.199	0.199	0.333	-0.266
0.875	-0.118	-0.118	-0.075	-0.173
1.216	0.201	0.201	-0.337	0.193
1.286	0.200	-0.200	0.153	0.319
1.540	0.212	0.212	-0.155	-0.200
1.701	0.322	-0.321	0.006	0.132
2.167	-0.086	-0.086	0.317	-0.355
2.499	-0.375	0.375	-0.331	0.275

Energi elektron π (sebelum tehnik w)
untuk krisena

$E_{\pi} = 18.0000\ \alpha + 25.1922\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)	q(17)	q(18)
1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.000	-0.000	-0.000	-0.000	0.000	0.000	-0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.000	0.000	-0.000	-0.000	0.000	0.000	0.000

f(15)	f(16)	f(17)	f(18)
-0.000	-0.000	0.000	0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 13)	(2 3)	(3 4)	(4 14)	(5 6)	(5 15)
0.712	0.568	0.617	0.707	0.583	0.754	0.538
(6 18)	(7 8)	(7 18)	(8 9)	(9 10)	(10 17)	(11 12)
0.521	0.712	0.568	0.617	0.707	0.583	0.754
(11 16)	(12 13)	(13 14)	(14 15)	(15 16)	(16 17)	(17 18)
0.538	0.521	0.535	0.476	0.573	0.476	0.535

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.451	0.403	0.408	0.442	0.440	0.457	0.451
Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.403	0.408	0.442	0.440	0.457	0.107	0.138
Fv(15)	Fv(16)	Fv(17)	Fv(18)			
0.145	0.145	0.138	0.107			

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.17	0.03	0.11	0.12	0.11	0.30	0.17
fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.03	0.11	0.12	0.11	0.30	0.00	0.02
fe(15)	fe(16)	fe(17)	fe(18)			
0.14	0.14	0.02	0.00			

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.17	0.03	0.11	0.12	0.11	0.30	0.17
fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.03	0.11	0.12	0.11	0.30	0.00	0.02
fn(15)	fn(16)	fn(17)	fn(18)			
0.14	0.14	0.02	0.00			

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.17	0.03	0.11	0.12	0.11	0.30	0.17

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.03	0.11	0.12	0.11	0.30	0.00	0.02

fr(15)	fr(16)	fr(17)	fr(18)
0.14	0.14	0.02	0.00

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.99	0.86	0.90	0.95	0.95	1.04	0.99

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.86	0.90	0.95	0.95	1.04	0.72	0.77

Se(15)	Se(16)	Se(17)	Se(18)
0.83	0.83	0.77	0.72

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.99	0.86	0.90	0.95	0.95	1.04	0.99

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.86	0.90	0.95	0.95	1.04	0.72	0.77

Sn(15)	Sn(16)	Sn(17)	Sn(18)
0.83	0.83	0.77	0.72

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.99	0.86	0.90	0.95	0.95	1.04	0.99

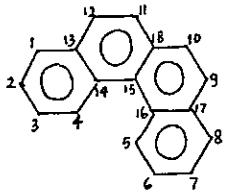
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.86	0.90	0.95	0.95	1.04	0.72	0.77

Sr(15)	Sr(16)	Sr(17)	Sr(18)
0.83	0.83	0.77	0.72

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LAMPIRAN VIII

HASIL PERHITUNGAN UNTUK MOLEKUL 3,4-BENZFENANTRENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk 3,4-benzfenantrena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.507	0.154	0.108	0.117	0.185	0.185	0.117	0.108
-2.136	0.279	0.232	0.218	0.232	-0.232	-0.218	-0.232
-1.769	0.218	0.279	0.276	0.209	0.209	0.276	0.279
-1.414	0.241	0.034	-0.194	-0.308	-0.034	0.194	0.308
-1.414	0.158	0.321	0.296	0.097	-0.321	-0.296	-0.097
-1.123	0.076	-0.255	-0.363	-0.153	-0.153	-0.363	-0.255
-1.000	0.354	0.354	0.000	-0.354	0.354	0.000	-0.354
-0.662	0.218	-0.092	-0.279	-0.093	0.092	0.279	0.092
-0.568	0.299	0.232	-0.168	-0.327	-0.327	-0.168	0.232
0.568	0.300	-0.231	-0.168	0.327	0.327	-0.168	-0.232
0.662	0.217	0.093	-0.278	0.092	-0.093	0.279	-0.092
1.000	0.354	-0.354	0.000	0.354	-0.354	-0.000	0.354
1.123	0.076	0.255	-0.363	0.153	0.153	-0.363	0.255
1.414	0.199	-0.322	0.256	-0.040	0.322	-0.256	0.040
1.414	0.209	0.024	-0.244	0.320	-0.024	0.244	-0.320
1.769	0.218	-0.279	0.276	-0.209	-0.209	0.276	-0.279
2.136	0.279	-0.232	0.218	-0.232	0.232	-0.218	0.232
2.507	0.154	-0.108	0.117	-0.185	-0.185	0.117	-0.108

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.507	0.154	0.194	0.209	0.209	0.194	0.277	0.348
-2.136	-0.279	-0.218	-0.102	0.102	0.218	0.363	0.279
-1.769	0.218	-0.124	-0.325	-0.325	-0.124	0.106	0.094
-1.414	0.241	0.047	0.034	0.308	0.435	0.308	-0.241
-1.414	0.158	0.454	0.321	-0.097	-0.137	-0.097	-0.158
-1.123	0.076	0.115	-0.212	-0.212	0.115	0.341	0.192
-1.000	-0.354	-0.000	-0.000	0.000	0.000	-0.000	-0.354
-0.662	-0.217	0.279	0.421	-0.421	-0.279	0.236	0.218
-0.568	0.300	-0.317	-0.119	-0.118	-0.317	-0.062	-0.018
0.568	0.299	-0.317	0.118	0.119	-0.317	0.061	-0.017
0.662	-0.218	0.279	-0.421	0.421	-0.278	-0.236	0.218
1.000	-0.354	0.000	0.000	-0.000	-0.000	0.000	-0.354
1.123	0.076	0.115	0.212	0.212	0.115	-0.341	0.192
1.414	0.199	0.455	-0.322	0.040	-0.057	0.040	-0.199
1.414	0.209	-0.035	0.024	-0.320	0.453	-0.320	-0.209
1.769	0.218	-0.124	0.325	0.325	-0.124	-0.106	0.094
2.136	-0.279	-0.218	0.102	-0.102	0.218	-0.363	0.279
2.507	0.154	0.194	-0.209	-0.209	0.194	-0.277	0.348

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X	C(15)	C(16)	C(17)	C(18)
-2.507	0.409	0.348	0.277	0.330
-2.136	0.000	-0.279	-0.363	-0.000
-1.769	-0.149	0.094	0.106	-0.452
-1.414	-0.341	-0.241	0.034	-0.000
-1.414	-0.224	-0.158	0.321	-0.000
-1.123	0.027	0.192	0.341	-0.353
-1.000	0.000	0.354	0.000	0.000
-0.662	0.000	-0.218	-0.236	0.000
-0.568	0.379	-0.017	-0.061	0.250
0.568	-0.379	-0.018	0.062	0.250
0.662	0.000	-0.218	0.236	-0.000
1.000	0.000	0.354	-0.000	0.000
1.123	-0.027	0.192	-0.341	-0.353
1.414	0.281	-0.199	-0.322	0.000
1.414	0.296	-0.209	0.024	0.000
1.769	0.149	0.094	-0.106	-0.452
2.136	0.000	-0.279	0.363	-0.000
2.507	-0.409	0.348	-0.277	0.330

Energi elektron π (sebelum tehnik w)
untuk 5,4- benzfenantrena

$E = 18.0000\ \alpha + 25.1875\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)	q(17)	q(18)
1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	-0.000	-0.000	-0.000	0.000	0.000	-0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.000	-0.000	0.000	-0.000	0.000	0.000	0.000

f(15)	f(16)	f(17)	f(18)
0.000	-0.000	-0.000	0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 13)	(2 3)	(3 4)	(4 14)	(5 6)	(5 16)
0.712	0.570	0.616	0.709	0.578	0.709	0.578
(6 7)	(7 8)	(8 17)	(9 10)	(9 17)	(10 18)	(11 12)
0.616	0.712	0.570	0.761	0.520	0.522	0.761
(11 18)	(12 13)	(13 14)	(14 15)	(15 16)	(15 18)	(16 17)
0.522	0.520	0.533	0.489	0.489	0.574	0.533

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.450	0.404	0.407	0.445	0.445	0.407	0.404
Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.450	0.451	0.448	0.449	0.451	0.110	0.132
Fv(15)	Fv(16)	Fv(17)	Fv(18)			
0.180	0.132	0.110	0.113			

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.18	0.11	0.06	0.21	0.21	0.06	0.11
fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.18	0.20	0.03	0.03	0.20	0.01	0.00
fe(15)	fe(16)	fe(17)	fe(18)			
0.29	0.00	0.01	0.12			

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.18	0.11	0.06	0.21	0.21	0.06	0.11
fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.18	0.20	0.03	0.03	0.20	0.01	0.00
fn(15)	fn(16)	fn(17)	fn(18)			
0.29	0.00	0.01	0.12			

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.18	0.11	0.06	0.21	0.21	0.06	0.11

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.18	0.20	0.03	0.03	0.20	0.01	0.00

fr(15)	fr(16)	fr(17)	fr(18)
0.29	0.00	0.01	0.12

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.98	0.88	0.89	0.97	0.97	0.89	0.88

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.98	1.00	0.98	0.98	1.00	0.73	0.76

Se(15)	Se(16)	Se(17)	Se(18)
0.90	0.76	0.73	0.76

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.98	0.88	0.89	0.97	0.97	0.89	0.88

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.98	1.00	0.98	0.98	1.00	0.73	0.76

Sn(15)	Sn(16)	Sn(17)	Sn(18)
0.90	0.76	0.73	0.76

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.98	0.88	0.89	0.97	0.97	0.89	0.88

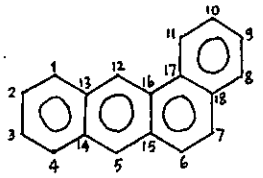
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.98	1.00	0.98	0.98	1.00	0.73	0.76

Sr(15)	Sr(16)	Sr(17)	Sr(18)
0.90	0.76	0.73	0.76

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LAMPIRAN IX

HASIL PERHITUNGAN UNTUK MOLEKUL TETRAFENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk tetrafena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.485	0.154	0.103	0.102	0.151	0.248	0.220	0.204
-2.176	0.267	0.230	0.233	0.276	0.173	-0.085	-0.194
-1.755	0.234	0.286	0.267	0.183	-0.213	-0.291	-0.084
-1.480	0.068	-0.122	-0.249	-0.246	-0.147	-0.340	-0.400
-1.323	0.319	0.326	0.113	-0.177	-0.378	0.067	0.241
-1.166	0.124	-0.273	-0.442	-0.242	0.011	-0.002	0.145
-1.000	0.316	0.316	0.000	-0.316	0.000	0.316	0.000
-0.715	0.196	-0.060	-0.238	-0.111	0.025	0.225	0.303
-0.452	0.301	0.236	-0.194	-0.324	0.445	-0.298	-0.288
0.452	0.300	-0.236	-0.194	0.324	-0.445	0.298	-0.288
0.715	0.196	0.060	-0.238	0.111	-0.025	-0.225	0.303
1.000	0.316	-0.316	-0.000	0.316	-0.000	-0.316	-0.000
1.166	0.123	0.273	-0.442	0.242	-0.011	0.002	0.145
1.323	0.319	-0.326	0.113	0.177	0.378	-0.067	0.241
1.480	0.068	0.122	-0.249	0.246	0.147	0.340	-0.400
1.755	0.234	-0.286	0.267	-0.183	0.213	0.291	-0.084
2.176	0.267	-0.230	0.233	-0.276	-0.173	0.085	-0.194
2.485	0.154	-0.103	0.102	-0.151	-0.248	-0.220	0.204

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.485	0.161	0.113	0.121	0.188	0.268	0.280	0.273
-2.176	-0.249	-0.205	-0.197	-0.224	0.130	0.352	0.368
-1.755	0.273	0.334	0.313	0.215	-0.069	0.125	0.054
-1.480	-0.195	-0.036	0.141	0.245	0.377	0.223	-0.115
-1.323	-0.050	-0.318	-0.371	-0.173	0.154	0.095	-0.347
-1.166	0.320	0.203	-0.084	-0.301	0.203	0.417	0.160
-1.000	-0.000	0.316	0.316	-0.000	-0.000	-0.000	-0.316
-0.715	-0.411	-0.285	0.208	0.434	-0.212	0.200	0.159
-0.452	0.160	-0.095	-0.203	0.003	-0.393	-0.100	0.047
0.452	0.160	0.095	-0.203	-0.003	-0.393	0.100	0.048
0.715	-0.411	0.285	0.208	-0.434	-0.212	-0.200	0.159
1.000	0.000	-0.316	0.316	0.000	-0.000	-0.000	-0.316
1.166	0.320	-0.203	-0.084	0.300	0.203	-0.417	0.160
1.323	-0.050	0.318	-0.371	0.173	0.155	-0.096	-0.347
1.480	-0.195	0.036	0.141	-0.245	0.377	-0.223	-0.115
1.755	0.273	-0.334	0.313	-0.215	-0.069	-0.125	0.054
2.176	-0.249	0.205	-0.197	0.224	0.130	-0.352	0.368
2.485	0.161	-0.113	0.121	-0.188	0.268	-0.280	0.273

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X	C(15)	C(16)	C(17)	C(18)
-2.485	0.344	0.385	0.346	0.286
-2.176	0.009	-0.069	-0.289	-0.337
-1.755	-0.428	-0.246	0.065	0.145
-1.480	-0.103	0.335	0.222	-0.252
-1.323	-0.153	0.109	0.142	0.252
-1.166	-0.147	-0.181	-0.267	0.170
-1.000	0.316	-0.000	-0.316	-0.316
-0.715	-0.142	-0.351	0.102	-0.009
-0.452	0.154	-0.078	0.204	0.167
0.452	0.154	0.078	0.204	-0.167
0.715	-0.142	0.351	0.102	0.009
1.000	0.316	0.000	-0.316	0.316
1.166	-0.147	0.181	-0.267	-0.170
1.323	-0.153	-0.109	0.142	-0.252
1.480	-0.103	-0.335	0.222	0.252
1.755	-0.428	0.246	0.065	-0.145
2.176	0.009	0.069	-0.289	0.336
2.485	0.344	-0.385	0.346	-0.286

Energi elektron π (sebelum tehnik w)
untuk tetrafena

$E = 18.0000\ \alpha + 25.1012\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)	q(17)	q(18)
1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.000	-0.000	0.000	-0.000	-0.000	-0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.000	-0.000	0.000	-0.000	0.000	-0.000	0.000

f(15)	f(16)	f(17)	f(18)
0.000	0.000	0.000	0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 13)	(2 3)	(3 4)	(4 14)	(5 14)	(5 15)
0.731	0.545	0.593	0.732	0.542	0.590	0.628

(6 7)	(6 15)	(7 18)	(8 9)	(8 18)	(9 10)	(10 11)
0.783	0.494	0.494	0.700	0.581	0.628	0.695

(11 17)	(12 13)	(12 16)	(13 14)	(15 16)	(16 17)	(17 18)
0.597	0.584	0.646	0.495	0.500	0.447	0.546

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.457	0.408	0.407	0.458	0.514	0.455	0.455

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.450	0.403	0.409	0.440	0.502	0.108	0.105

Fv(15)	Fv(16)	Fv(17)	Fv(18)
0.111	0.140	0.142	0.111

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.18	0.11	0.08	0.21	0.40	0.18	0.17

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.05	0.02	0.08	0.00	0.31	0.02	0.00

fe(15)	fe(16)	fe(17)	fe(18)
0.05	0.01	0.08	0.06

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.18	0.11	0.08	0.21	0.40	0.18	0.17

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.05	0.02	0.08	0.00	0.31	0.02	0.00

fn(15)	fn(16)	fn(17)	fn(18)
0.05	0.01	0.08	0.06

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.18	0.11	0.08	0.21	0.40	0.18	0.17

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.05	0.02	0.08	0.00	0.31	0.02	0.00

fr(15)	fr(16)	fr(17)	fr(18)
0.05	0.01	0.08	0.06

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
1.04	0.91	0.90	1.05	1.25	1.04	1.04

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.98	0.87	0.91	0.93	1.19	0.73	0.71

Se(15)	Se(16)	Se(17)	Se(18)
0.75	0.79	0.81	0.75

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.04	0.91	0.90	1.05	1.25	1.04	1.04

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.98	0.87	0.91	0.93	1.19	0.73	0.71

Sn(15)	Sn(16)	Sn(17)	Sn(18)
0.75	0.79	0.81	0.75

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.04	0.91	0.90	1.05	1.25	1.04	1.04

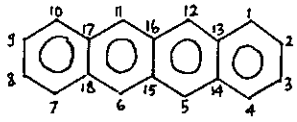
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.98	0.87	0.91	0.93	1.19	0.73	0.71

Sr(15)	Sr(16)	Sr(17)	Sr(18)
0.75	0.79	0.81	0.75

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LAMPIRAN X

HASIL PERHITUNGAN UNTUK MOLEKUL TETRASENA



Hasil perhitungan koefisien orbital molekul Huckel
(sebelum tehnik w) untuk tetrasena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.467	0.161	0.109	0.109	0.161	0.260	0.260	0.160
-2.194	0.252	0.212	0.212	0.252	0.156	-0.156	-0.252
-1.777	0.235	0.302	0.302	0.235	-0.145	-0.145	0.235
-1.467	0.208	0.084	-0.084	-0.208	-0.337	-0.337	-0.208
-1.295	0.113	0.384	0.384	0.113	-0.183	0.183	-0.113
-1.194	0.342	0.156	-0.156	-0.342	-0.212	0.211	0.342
-1.000	0.000	0.316	0.316	0.000	-0.000	0.000	-0.000
-0.777	0.355	0.200	-0.200	-0.355	0.219	0.219	-0.355
-0.295	0.237	0.183	-0.183	-0.237	0.384	-0.384	0.237
0.295	0.237	-0.183	-0.183	0.237	-0.384	0.384	-0.237
0.777	0.355	-0.200	-0.199	0.355	-0.219	-0.219	0.355
1.000	0.000	0.316	-0.316	0.000	-0.000	-0.000	0.000
1.194	0.342	-0.156	-0.156	0.342	0.212	-0.212	-0.342
1.295	0.113	-0.384	0.384	-0.113	0.183	-0.183	0.113
1.467	0.208	-0.084	-0.084	0.208	0.337	0.337	0.208
1.777	0.235	-0.302	0.302	-0.235	0.145	0.145	-0.235
2.194	0.252	-0.211	0.211	-0.252	-0.156	0.156	0.253
2.467	0.161	-0.109	0.109	-0.161	-0.260	-0.260	-0.161

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.467	0.109	0.109	0.160	0.260	0.260	0.287	0.287
-2.194	-0.212	-0.212	-0.253	-0.156	0.156	0.342	0.342
-1.777	0.302	0.302	0.235	-0.145	-0.145	0.115	0.115
-1.467	-0.085	0.084	0.208	0.337	0.337	0.221	-0.221
-1.295	-0.384	-0.384	-0.113	0.183	-0.183	-0.237	-0.237
-1.194	0.156	-0.156	-0.342	-0.211	0.212	0.252	-0.252
-1.000	0.316	0.316	-0.000	0.000	-0.000	-0.316	-0.316
-0.777	-0.200	0.199	0.355	-0.219	-0.219	0.076	-0.076
-0.295	0.183	-0.183	-0.237	0.384	-0.384	-0.113	0.113
0.295	0.183	0.183	-0.237	0.384	-0.384	0.113	0.113
0.777	-0.199	-0.200	0.355	-0.219	-0.219	-0.076	-0.076
1.000	-0.316	0.316	0.000	-0.000	-0.000	-0.316	0.316
1.194	0.156	0.156	-0.342	-0.211	0.212	-0.252	-0.253
1.295	-0.384	0.384	-0.113	0.183	-0.183	0.237	-0.237
1.467	-0.084	-0.084	0.208	0.337	0.337	-0.221	-0.221
1.777	0.302	-0.302	0.234	-0.145	-0.145	-0.115	0.115
2.194	-0.212	0.212	-0.253	-0.156	0.156	-0.342	0.342
2.467	0.109	-0.109	0.161	0.260	0.260	-0.286	0.287

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X	C(15)	C(16)	C(17)	C(18)
-2.467	0.354	0.354	0.287	0.287
-2.194	0.000	-0.000	-0.342	-0.342
-1.777	-0.373	-0.373	0.115	0.115
-1.467	-0.273	0.273	0.221	-0.221
-1.295	-0.000	-0.000	0.237	0.237
-1.194	-0.000	0.000	-0.252	0.253
-1.000	0.316	0.316	-0.316	-0.316
-0.777	0.247	-0.247	0.076	-0.076
-0.295	-0.000	0.000	0.113	-0.113
0.295	-0.000	-0.000	-0.113	-0.113
0.777	0.247	0.247	-0.076	-0.076
1.000	-0.316	0.316	-0.316	0.316
1.194	-0.000	-0.000	0.252	0.252
1.295	-0.000	0.000	-0.237	0.237
1.467	-0.273	-0.273	-0.221	-0.221
1.777	-0.373	0.373	-0.115	0.115
2.194	0.000	-0.000	0.342	-0.342
2.467	0.354	-0.354	-0.287	0.287

Energi elektron π (sebelum tehnik w)
untuk tetrasena

$E = 18.0000\ \alpha + 24.9308\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)	q(17)	q(18)
1.000	1.000	1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.000	-0.000	-0.000	0.000	0.000	0.000	0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.000	-0.000	0.000	-0.000	-0.000	-0.000	0.000

f(15)	f(16)	f(17)	f(18)
0.000	-0.000	-0.000	0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 13)	(2 3)	(3 4)	(4 14)	(5 14)	(5 15)
0.741	0.530	0.581	0.741	0.530	0.618	0.584

(6 15)	(6 18)	(7 8)	(7 18)	(8 9)	(9 10)	(10 17)
0.584	0.618	0.741	0.530	0.581	0.741	0.530

(11 16)	(11 17)	(12 13)	(12 16)	(13 14)	(15 16)	(17 18)
0.584	0.618	0.618	0.584	0.475	0.458	0.475

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.461	0.410	0.410	0.461	0.529	0.529	0.461

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.410	0.410	0.461	0.529	0.529	0.108	0.108

Fv(15)	Fv(16)	Fv(17)	Fv(18)
0.105	0.105	0.108	0.108

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.11	0.07	0.07	0.11	0.29	0.29	0.11

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.07	0.07	0.11	0.29	0.29	0.03	0.03

fe(15)	fe(16)	fe(17)	fe(18)
0.00	0.00	0.03	0.03

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.11	0.07	0.07	0.11	0.29	0.29	0.11

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.07	0.07	0.11	0.29	0.29	0.03	0.03

fn(15)	fn(16)	fn(17)	fn(18)
0.00	0.00	0.03	0.03

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.11	0.07	0.07	0.11	0.29	0.29	0.11

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.07	0.07	0.11	0.29	0.29	0.03	0.03

fr(15)	fr(16)	fr(17)	fr(18)
0.00	0.00	0.03	0.03

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
1.12	0.96	0.96	1.12	1.50	1.50	1.12

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.96	0.96	1.12	1.51	1.50	0.75	0.75

Se(15)	Se(16)	Se(17)	Se(18)
0.72	0.72	0.75	0.75

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.12	0.96	0.96	1.12	1.50	1.50	1.12

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.96	0.96	1.12	1.50	1.50	0.75	0.75

Sn(15)	Sn(16)	Sn(17)	Sn(18)
0.72	0.72	0.75	0.75

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.12	0.96	0.96	1.12	1.50	1.50	1.12

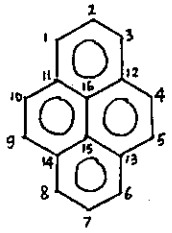
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.96	0.96	1.12	1.50	1.50	0.75	0.75

Sr(15)	Sr(16)	Sr(17)	Sr(18)
0.72	0.72	0.75	0.75

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LAMPIRAN XI

HASIL PERHITUNGAN UNTUK MOLEKUL PIRENA



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk pirena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.532	0.174	0.138	0.174	0.198	0.198	0.174	0.138
-2.000	0.297	0.297	0.297	0.099	-0.099	-0.297	-0.297
-1.802	0.164	-0.000	-0.164	-0.368	-0.368	-0.164	-0.000
-1.347	0.311	0.461	0.311	-0.123	-0.123	0.311	0.461
-1.247	0.295	-0.000	-0.296	-0.164	0.164	0.296	0.000
-1.000	0.000	-0.000	0.000	-0.408	-0.408	-0.000	-0.000
-0.879	0.187	0.424	0.186	-0.138	0.138	-0.186	-0.424
-0.445	0.368	-0.000	-0.368	0.296	0.295	-0.368	0.000
0.445	0.368	0.000	-0.369	0.296	-0.295	0.368	0.000
0.879	0.187	-0.424	0.186	-0.138	-0.138	0.186	-0.424
1.000	0.000	-0.000	-0.000	0.408	-0.408	0.000	-0.000
1.247	0.295	0.000	-0.296	-0.164	-0.164	-0.296	0.000
1.347	0.311	-0.461	0.311	-0.123	0.123	-0.311	0.461
1.802	0.164	0.000	-0.164	-0.368	0.369	0.164	-0.000
2.000	0.297	-0.297	0.297	0.099	0.099	0.297	-0.297
2.532	0.174	-0.138	0.174	0.198	-0.198	-0.174	0.138

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.532	0.174	0.198	0.198	0.304	0.304	0.304	0.304
-2.000	-0.297	-0.099	0.099	0.297	0.297	-0.297	-0.297
-1.802	0.164	0.368	0.369	0.295	-0.296	-0.296	0.296
-1.347	0.311	-0.123	-0.123	-0.043	-0.043	-0.043	-0.043
-1.247	-0.295	-0.164	0.164	0.368	-0.368	0.368	-0.369
-1.000	-0.000	-0.408	-0.408	0.000	0.000	-0.000	0.000
-0.879	-0.187	0.138	-0.138	-0.260	-0.260	0.260	0.260
-0.445	0.369	-0.296	-0.295	0.164	-0.164	-0.164	0.164
0.445	-0.368	0.296	-0.295	-0.164	0.164	-0.164	0.164
0.879	0.187	-0.138	-0.138	0.260	0.260	0.260	0.260
1.000	0.000	-0.408	0.408	-0.000	0.000	0.000	-0.000
1.247	0.295	0.164	0.164	-0.369	0.368	0.368	-0.368
1.347	-0.311	0.123	-0.123	0.043	0.043	-0.043	-0.043
1.802	-0.164	-0.369	0.368	-0.295	0.295	-0.296	0.296
2.000	0.297	0.099	0.099	-0.297	-0.297	-0.297	-0.297
2.532	-0.174	-0.198	0.198	-0.304	-0.304	0.304	0.304

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X	C(15)	C(16)
-2.532	0.396	0.396
-2.000	-0.198	0.198
-1.802	0.000	0.000
-1.347	-0.245	-0.245
-1.247	-0.000	0.000
-1.000	0.408	0.408
-0.879	0.277	-0.277
-0.445	0.000	-0.000
0.445	0.000	0.000
0.879	-0.277	-0.277
1.000	0.408	-0.408
1.247	0.000	0.000
1.347	0.245	-0.245
1.802	-0.000	0.000
2.000	0.198	0.198
2.532	-0.396	0.396

Energi elektron π (sebelum tehnik w)
untuk pirena

$E = 16.0000\ \alpha + 22.5055\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.000	1.000	1.000	1.000	1.000	1.000	1.000

q(15)	q(16)
1.000	1.000

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
-0.000	0.000	0.000	-0.000	0.000	0.000	-0.000

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.000	-0.000	-0.000	0.000	-0.000	-0.000	-0.000

f(15)	f(16)
-0.000	-0.000

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 11)	(2 3)	(3 12)	(4 5)	(4 12)	(5 13)
0.669	0.594	0.669	0.594	0.777	0.503	0.504

(6 7)	(6 13)	(7 8)	(8 14)	(9 10)	(9 14)	(10 11)
0.669	0.594	0.670	0.594	0.777	0.503	0.503

(11 16)	(12 16)	(13 15)	(14 15)	(15 16)
0.524	0.523	0.523	0.524	0.536

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.468	0.393	0.468	0.452	0.452	0.468	0.393

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.468	0.452	0.452	0.111	0.111	0.111	0.111

Fv(15)	Fv(16)
0.149	0.149

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.27	0.00	0.27	0.17	0.17	0.27	0.00

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.27	0.17	0.17	0.05	0.05	0.05	0.05

fe(15)	fe(16)
0.00	0.00

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.27	0.00	0.27	0.17	0.17	0.27	0.00

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.27	0.17	0.17	0.05	0.05	0.05	0.05

fn(15)	fn(16)
0.00	0.00

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.27	0.00	0.27	0.17	0.17	0.27	0.00

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.27	0.17	0.17	0.05	0.05	0.05	0.05

fr(15)	fr(16)
0.00	0.00

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
1.11	0.83	1.11	1.03	1.03	1.11	0.83

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
1.11	1.03	1.03	0.75	0.75	0.75	0.75

Se(15)	Se(16)
0.76	0.76

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.11	0.83	1.11	1.03	1.03	1.11	0.83

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
1.11	1.03	1.03	0.75	0.75	0.75	0.75

Sn(15)	Sn(16)
0.76	0.76

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.11	0.83	1.11	1.03	1.03	1.11	0.83

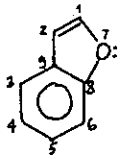
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
1.11	1.03	1.03	0.75	0.75	0.75	0.75

Sr(15)	Sr(16)
0.76	0.76

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LAMPIRAN XII

HASIL PERHITUNGAN UNTUK MOLEKUL KUMARIN



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk kumarin

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.721	0.301	0.208	0.128	0.082	0.095	0.177	0.763
-1.898	0.111	-0.149	-0.429	-0.422	-0.372	-0.285	0.449
-1.353	0.259	0.513	0.170	-0.205	-0.447	-0.400	-0.203
-0.893	0.161	-0.051	0.366	0.534	0.111	-0.434	0.244
-0.621	0.536	0.470	-0.380	0.008	0.385	0.231	-0.171
0.808	0.539	-0.290	0.437	-0.049	-0.398	0.370	-0.182
1.083	0.167	-0.030	-0.385	0.552	-0.213	-0.322	-0.189
1.449	0.431	-0.528	-0.041	-0.275	0.440	-0.362	-0.120
2.148	0.113	-0.290	-0.389	0.325	-0.308	0.338	0.058

X	C(8)	C(9)
-2.721	0.387	0.266
-1.898	-0.168	-0.393
-1.353	-0.094	0.435
-0.893	-0.499	-0.207
-0.621	-0.241	-0.244
0.808	0.099	-0.305
1.083	0.561	-0.135
1.449	0.085	0.335
2.148	-0.417	0.510

Energi elektron π (sebelum tehnik w) untuk kumarin

$E = 10.0000\ \alpha + 14.9744\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.966	1.103	1.015	1.024	1.016	1.029	1.827

q(8)	q(9)
0.989	1.033

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Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.034	-0.103	-0.015	-0.024	-0.016	-0.029	0.173

f(8)	f(9)
0.011	-0.033

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 7)	(2 9)	(3 4)	(3 9)	(4 5)	(5 6)
0.844	0.349	0.465	0.698	0.587	0.638	0.684

(6 8)	(7 8)	(8 9)
0.631	0.317	0.580

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.539	0.423	0.447	0.396	0.410	0.417	2.066

Fv(8)	Fv(9)
0.204	0.100

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.57	0.44	0.29	0.00	0.30	0.11	0.06

fe(8)	fe(9)
0.12	0.12

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.58	0.17	0.38	0.00	0.32	0.27	0.07

fn(8)	fn(9)
0.02	0.19

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.58	0.30	0.34	0.00	0.31	0.19	0.06

fr(8)	fr(9)
0.07	0.15

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
1.16	1.16	1.01	0.89	0.95	0.94	0.93

Se(8)	Se(9)
0.90	0.78

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.04	0.67	0.89	0.77	0.83	0.82	0.17

Sn(8)	Sn(9)
0.78	0.66

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

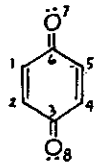
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.10	0.92	0.95	0.83	0.89	0.88	0.55

Sr(8)	Sr(9)
0.84	0.72

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LAMPIRAN XIII

HASIL PERHITUNGAN UNTUK MOLEKUL BENZOKUINON



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk benzokuinon

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.675	0.214	0.214	0.358	0.214	0.214	0.358	0.530
-2.514	0.090	-0.090	-0.318	-0.090	0.090	0.318	0.618
-1.539	0.370	0.370	0.199	0.370	0.370	0.199	-0.433
-1.000	0.500	0.500	-0.000	-0.500	-0.500	0.000	-0.000
-0.572	0.297	-0.297	-0.466	-0.297	0.297	0.466	-0.326
1.000	0.500	-0.500	0.000	0.500	-0.500	0.000	-0.000
1.214	0.261	0.260	-0.576	0.261	0.260	-0.576	0.179
2.086	0.392	-0.392	0.426	-0.392	0.392	-0.426	0.104

X	C(8)
-2.675	0.530
-2.514	-0.618
-1.539	-0.432
-1.000	0.000
-0.572	0.327
1.000	-0.000
1.214	0.179
2.086	-0.104

Energi elektron π (sebelum tehnik w) untuk benzokuinon

$E = 8.0000\ \alpha + 15.4569\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.881	0.881	0.538	0.881	0.881	0.538	1.701

q(8)
1.701

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Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.119	0.119	0.462	0.119	0.119	0.462	-0.701

f(8)
-0.701

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 6)	(2 3)	(3 4)	(3 8)	(4 5)	(5 6)
0.848	0.358	0.358	0.358	0.600	0.848	0.358

(6 7)
0.600

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.526	0.526	0.417	0.526	0.526	0.417	3.132

Fv(8)
3.132

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.50	0.50	0.00	0.50	0.50	0.00	0.00

fe(8)
0.00

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.18	0.18	0.43	0.18	0.18	0.43	0.21

fn(8)
0.21

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)	fr(8)
0.34	0.34	0.22	0.34	0.34	0.22	0.11	0.11

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)	Se(8)
0.72	0.72	0.23	0.72	0.72	0.23	0.76	0.76

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)	Sn(8)
0.45	0.45	-0.04	0.45	0.45	-0.04	-0.31	-0.31

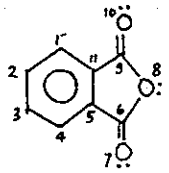
Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)	Sr(8)
0.58	0.58	0.09	0.58	0.58	0.09	0.22	0.22

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LAMPIRAN XIV

HASIL PERHITUNGAN UNTUK MOLEKUL FTALAT ANHIDRAT



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk ftalat anhidrat

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.944	0.086	0.044	0.044	0.086	0.208	0.354	0.375
-2.457	0.040	0.012	-0.012	-0.040	-0.088	-0.291	-0.637
-2.000	0.009	0.009	0.009	0.009	0.009	-0.000	0.526
-2.000	0.386	0.386	0.386	0.386	0.386	-0.000	-0.164
-1.104	0.052	0.503	0.503	0.052	-0.445	-0.110	0.122
-1.072	0.540	0.261	-0.261	-0.540	-0.319	-0.133	0.144
0.051	0.227	0.239	-0.239	-0.227	0.250	0.516	-0.251
0.711	0.461	-0.270	-0.269	0.461	-0.058	-0.402	0.148
1.304	0.161	-0.530	0.531	-0.162	-0.320	0.287	-0.087
1.337	0.358	-0.153	-0.153	0.358	-0.326	0.448	-0.134
2.174	0.359	-0.306	0.306	-0.359	0.475	-0.221	0.053

X	C(8)	C(9)	C(10)	C(11)
-2.944	0.601	0.355	0.376	0.208
-2.457	-0.000	0.291	0.637	0.087
-2.000	-0.668	-0.000	0.526	0.009
-2.000	-0.229	0.000	-0.164	0.386
-1.104	0.196	-0.110	0.122	-0.445
-1.072	0.000	0.133	-0.144	0.319
0.051	0.000	-0.516	0.251	-0.250
0.711	0.237	-0.402	0.148	-0.058
1.304	0.000	-0.287	0.087	0.320
1.337	-0.215	0.448	-0.134	-0.326
2.174	-0.000	0.221	-0.053	-0.475

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Energi elektron π (sebelum tehnik w)
untuk ftalat anhidrat

E = 12.0000 α +23.1555 β

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.905	0.944	0.944	0.905	0.999	0.481	1.773

q(8)	q(9)	q(10)	q(11)
1.795	0.481	1.773	0.999

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.095	0.056	0.056	0.095	0.001	0.519	-0.773

f(8)	f(9)	f(10)	f(11)
0.205	0.519	-0.773	0.001

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 11)	(2 3)	(3 4)	(4 5)	(5 6)	(5 11)
0.641	0.639	0.672	0.641	0.639	0.381	0.562

(6 7)	(6 8)	(8 9)	(9 10)	(9 11)
0.572	0.383	0.383	0.572	0.381

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.452	0.419	0.419	0.452	0.150	0.395	3.160

Fv(8)	Fv(9)	Fv(10)	Fv(11)
1.966	0.395	3.160	0.150

Indeks kereaktifan (frontier orbital) terhadap elektrofil
(sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.58	0.14	0.14	0.58	0.20	0.04	0.04

fe(8)	fe(9)	fe(10)	fe(11)
0.00	0.04	0.04	0.20

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Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.10	0.11	0.11	0.10	0.13	0.53	0.13

fn(8)	fn(9)	fn(10)	fn(11)
0.00	0.53	0.13	0.13

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.34	0.12	0.13	0.34	0.16	0.28	0.08

fr(8)	fr(9)	fr(10)	fr(11)
0.00	0.28	0.08	0.16

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.70	0.74	0.74	0.70	0.73	0.21	0.80

Se(8)	Se(9)	Se(10)	Se(11)
0.81	0.21	0.80	0.73

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
2.97	3.00	3.00	2.97	3.00	11.38	2.59

Sn(8)	Sn(9)	Sn(10)	Sn(11)
0.23	11.38	2.59	3.00

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

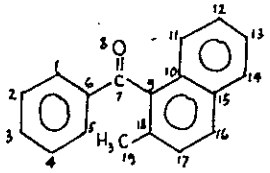
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.84	1.87	1.87	1.84	1.86	5.80	1.69

Sr(8)	Sr(9)	Sr(10)	Sr(11)
0.52	5.80	1.69	1.86

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LAMPIRAN XV

HASIL PERHITUNGAN UNTUK MOLEKUL 1-BENZOIL-2-METILNAFTALENA



Hasil perhitungan koefisien orbital molekul Huckel
(sebelum tehnik w) untuk 1-benzoil-2-metilnaftalena

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.636	0.114	0.061	0.046	0.061	0.114	0.240	0.449
-2.291	0.061	0.043	0.037	0.043	0.061	0.096	0.110
-2.000	0.383	0.383	0.383	0.383	0.383	0.383	0.000
-1.735	0.020	0.034	0.039	0.034	0.020	0.000	-0.044
-1.367	0.009	-0.090	-0.132	-0.090	0.009	0.102	0.136
-1.136	0.133	-0.212	-0.375	-0.213	0.133	0.364	0.163
-1.089	0.152	-0.203	-0.373	-0.203	0.152	0.368	0.108
-1.000	0.500	0.500	0.000	-0.500	-0.500	-0.000	-0.000
-0.707	0.096	-0.045	-0.127	-0.045	0.095	0.112	-0.124
-0.179	0.164	-0.015	-0.167	-0.015	0.164	0.044	-0.356
0.367	0.236	0.046	-0.253	0.046	0.236	-0.133	-0.470
0.736	0.168	0.085	-0.231	0.085	0.168	-0.209	-0.203
1.000	0.500	-0.500	0.000	0.500	-0.500	-0.000	0.000
1.099	0.073	0.101	-0.184	0.101	0.073	-0.182	0.059
1.206	0.104	0.230	-0.381	0.230	0.104	-0.355	0.245
1.468	0.023	-0.213	0.290	-0.213	0.022	0.180	-0.343
1.767	0.092	-0.145	0.164	-0.145	0.092	-0.018	-0.170
2.100	0.376	-0.327	0.312	-0.327	0.376	-0.462	0.242
2.397	0.094	-0.060	0.050	-0.060	0.094	-0.166	0.232

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.636	0.705	0.291	0.197	0.095	0.054	0.046	0.068
-2.291	0.379	-0.236	-0.402	-0.266	-0.208	-0.210	-0.274
-2.000	-0.345	-0.000	0.000	-0.000	-0.000	0.000	-0.000
-1.735	0.165	-0.267	0.067	0.246	0.360	0.379	0.297
-1.367	-0.215	0.343	0.254	0.366	0.247	-0.028	-0.286
-1.136	-0.189	0.052	0.221	-0.099	-0.334	-0.280	0.016
-1.089	-0.119	-0.105	-0.398	-0.157	0.227	0.404	0.213
-1.000	0.000	0.000	-0.000	-0.000	0.000	0.000	0.000
-0.707	0.096	-0.316	0.001	0.421	0.296	-0.212	-0.446
-0.179	0.196	-0.333	0.132	0.163	-0.103	-0.181	0.071
0.367	0.199	0.104	0.192	-0.027	-0.182	0.093	0.148
0.736	0.074	0.293	0.045	-0.416	0.261	0.224	-0.426
1.000	-0.000	0.000	0.000	-0.000	-0.000	0.000	-0.000
1.099	-0.019	0.130	-0.473	0.134	0.325	-0.492	0.215
1.206	-0.076	0.111	-0.068	0.297	-0.291	0.054	0.226
1.468	0.099	0.270	-0.189	0.278	-0.219	0.044	0.155
1.767	0.045	0.302	0.068	-0.233	0.344	-0.375	0.319
2.100	-0.059	-0.038	-0.123	0.112	-0.112	0.123	-0.147
2.397	-0.053	-0.393	0.429	-0.252	0.176	-0.169	0.230

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X	C(15)	C(16)	C(17)	C(18)	C(19)
-2.636	0.134	0.087	0.096	0.166	0.057
-2.291	-0.418	-0.282	-0.227	-0.239	-0.094
-2.000	0.000	-0.000	0.000	0.000	-0.000
-1.735	0.137	-0.126	-0.356	-0.492	-0.255
-1.367	-0.362	-0.463	-0.271	0.093	0.061
-1.136	0.298	0.101	-0.183	-0.309	-0.245
-1.089	-0.172	-0.002	0.169	0.186	0.154
-1.000	-0.000	-0.000	-0.000	0.000	0.000
-0.707	-0.104	0.372	0.366	-0.113	-0.144
-0.179	0.194	-0.169	-0.224	0.128	0.644
0.367	-0.148	-0.286	0.252	0.193	-0.474
0.736	0.090	0.314	-0.321	-0.078	0.095
1.000	-0.000	0.000	0.000	-0.000	-0.000
1.099	0.255	-0.023	-0.230	0.276	-0.226
1.206	-0.327	0.236	0.042	-0.287	0.214
1.468	-0.271	0.431	-0.363	0.101	-0.062
1.767	-0.188	-0.054	0.284	-0.448	0.228
2.100	0.185	-0.118	0.063	-0.015	0.006
2.397	-0.382	0.257	-0.235	0.305	-0.114

Energi elektron π (sebelum tehnik w)
untuk 1-benzoil-2-metilnaftalena

$E = 18.0000\ \alpha + 27.9224\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.928	1.000	0.930	1.000	0.928	1.009	0.576

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.785	0.887	0.953	0.972	0.975	0.954	0.989

q(15)	q(16)	q(17)	q(18)	q(19)
0.943	0.931	0.914	0.956	0.370

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.072	-0.000	0.070	-0.000	0.072	-0.009	0.424

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.785	0.113	0.047	0.028	0.025	0.046	0.011

f(15)	f(16)	f(17)	f(18)	f(19)
0.057	0.069	0.086	0.044	-0.370

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 6)	(2 3)	(3 4)	(4 5)	(5 6)	(6 7)
0.686	0.592	0.651	0.651	0.686	0.592	0.435
(7 8)	(7 9)	(9 10)	(9 18)	(10 11)	(10 15)	(11 12)
0.533	0.399	0.549	0.537	0.552	0.491	0.723
(12 13)	(13 14)	(14 15)	(15 16)	(16 17)	(17 18)	(18 19)
0.596	0.715	0.565	0.544	0.720	0.534	0.567

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.454	0.395	0.429	0.395	0.454	0.113	0.366
Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
3.199	0.248	0.140	0.457	0.413	0.420	0.452
Fv(15)	Fv(16)	Fv(17)	Fv(18)	Fv(19)		
0.132	0.468	0.479	0.095	0.165		

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.02	0.00	0.03	0.00	0.02	0.03	0.03
fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.02	0.20	0.00	0.35	0.18	0.09	0.40
fe(15)	fe(16)	fe(17)	fe(18)	fe(19)		
0.02	0.28	0.27	0.03	0.04		

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.05	0.00	0.06	0.00	0.05	0.00	0.25
fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.08	0.22	0.04	0.05	0.02	0.07	0.01
fn(15)	fn(16)	fn(17)	fn(18)	fn(19)		
0.08	0.06	0.10	0.03	0.83		

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.04	0.00	0.04	0.00	0.04	0.01	0.14

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.05	0.21	0.02	0.20	0.10	0.08	0.20

fr(15)	fr(16)	fr(17)	fr(18)	fr(19)
0.05	0.17	0.18	0.03	0.44

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.76	0.83	0.73	0.83	0.76	0.73	0.30

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.84	0.68	0.65	0.90	0.82	0.77	0.94

Se(15)	Se(16)	Se(17)	Se(18)	Se(19)
0.62	0.82	0.80	0.63	0.30

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.76	0.83	0.73	0.83	0.76	0.73	0.30

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
-0.16	-0.56	0.65	0.59	0.82	0.46	0.94

Sn(15)	Sn(16)	Sn(17)	Sn(18)	Sn(19)
0.31	0.82	0.49	0.63	-3.13

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.76	0.83	0.73	0.83	0.76	0.73	0.30

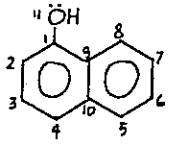
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.34	0.06	0.65	0.74	0.82	0.62	0.94

Sr(15)	Sr(16)	Sr(17)	Sr(18)	Sr(19)
0.47	0.82	0.64	0.63	-1.42

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LAMPIRAN XVI

HASIL PERHITUNGAN UNTUK MOLEKUL 1-NAFTOL



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk 1-naftol

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.658	0.471	0.227	0.133	0.126	0.102	0.069	0.081
-2.118	0.057	-0.048	-0.158	-0.286	-0.349	-0.291	-0.267
-1.565	0.082	0.366	0.490	0.401	-0.137	-0.352	-0.414
-1.164	0.259	0.233	0.013	-0.218	-0.470	-0.280	0.144
-1.000	0.000	0.408	0.408	-0.000	-0.000	0.408	0.408
-0.498	0.400	0.365	-0.218	-0.474	0.365	0.200	-0.265
0.683	0.401	-0.188	-0.273	0.374	-0.450	0.290	0.252
1.000	0.000	-0.408	0.408	-0.000	0.000	0.408	-0.408
1.352	0.403	-0.113	-0.251	0.452	0.347	-0.109	-0.200
1.641	0.321	-0.428	0.382	-0.199	0.300	-0.438	0.418
2.326	0.339	-0.245	0.231	-0.292	-0.286	0.218	-0.220

X	C(8)	C(9)	C(10)	C(11)
-2.658	0.147	0.308	0.202	0.717
-2.118	-0.275	-0.315	-0.449	0.483
-1.565	-0.296	-0.049	0.138	-0.189
-1.164	0.448	0.378	-0.267	-0.310
-1.000	0.000	-0.408	-0.408	-0.000
-0.498	-0.332	0.100	-0.018	-0.266
0.683	-0.462	0.064	0.017	-0.150
1.000	-0.000	0.408	-0.408	-0.000
1.352	0.379	-0.312	-0.360	-0.120
1.641	-0.248	-0.010	-0.055	-0.088
2.326	0.294	-0.465	0.448	-0.078

Energi elektron π (sebelum tehnik w) untuk 1-naftol

$E = 10.0000\ \alpha + 17.0089\ \beta$

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Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.598	0.818	0.899	0.613	0.745	0.918	0.874

q(8)	q(9)	q(10)	q(11)
0.770	1.011	0.998	1.757

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.402	0.182	0.101	0.387	0.255	0.082	0.126

f(8)	f(9)	f(10)	f(11)
0.230	-0.011	0.002	-1.757

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 9)	(1 11)	(2 3)	(3 4)	(4 10)	(5 6)
0.390	0.442	0.539	0.773	0.511	0.535	0.578

(5 10)	(6 7)	(7 8)	(8 9)	(9 10)
0.568	0.711	0.544	0.630	0.525

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.361	0.569	0.448	0.686	0.586	0.443	0.476

Fv(8)	Fv(9)	Fv(10)	Fv(11)
0.557	0.134	0.104	2.193

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.00	0.33	0.33	0.00	0.00	0.33	0.33

fe(8)	fe(9)	fe(10)	fe(11)
0.00	0.33	0.33	0.00

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Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.32	0.27	0.09	0.45	0.27	0.08	0.14

fn(8)	fn(9)	fn(10)	fn(11)
0.22	0.02	0.00	0.14

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.16	0.30	0.21	0.22	0.13	0.21	0.24

fr(8)	fr(9)	fr(10)	fr(11)
0.11	0.18	0.17	0.07

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.29	0.64	0.68	0.38	0.53	0.71	0.66

Se(8)	Se(9)	Se(10)	Se(11)
0.54	0.75	0.70	0.82

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.29	0.19	0.68	-0.07	0.42	0.71	0.55

Sn(8)	Sn(9)	Sn(10)	Sn(11)
0.54	0.64	0.70	-0.18

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

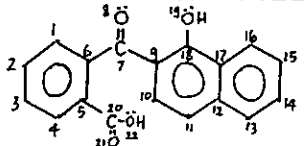
Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.29	0.42	0.68	0.15	0.47	0.71	0.60

Sr(8)	Sr(9)	Sr(10)	Sr(11)
0.54	0.69	0.70	0.32

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LAMPIRAN XVII

HASIL PERHITUNGAN UNTUK MOLEKUL ASAM 1-HIDROKSI-2-NAFTOIL-o-BENZOAT



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk asam 1-hidroksi-2-naftoil-o-benzoat

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.742	0.089	0.055	0.061	0.113	0.249	0.190	0.203
-2.645	0.056	0.024	0.007	-0.006	-0.023	0.126	0.332
-2.461	0.078	0.045	0.033	0.037	0.057	0.146	0.250
-2.104	0.004	0.003	0.003	0.003	0.004	0.005	0.003
-2.000	0.001	0.001	0.001	0.001	0.001	0.001	0.000
-2.000	0.370	0.370	0.370	0.370	0.370	0.370	0.000
-1.606	0.020	0.058	0.074	0.060	0.023	-0.027	-0.095
-1.242	0.035	-0.171	-0.247	-0.137	0.078	0.215	0.170
-1.147	0.011	-0.336	-0.396	-0.118	0.260	0.348	0.142
-1.075	0.448	0.430	0.015	-0.414	-0.460	0.051	0.074
-1.000	0.316	0.000	-0.316	-0.316	-0.000	0.316	-0.000
-0.583	0.097	-0.005	-0.099	-0.053	0.068	0.061	-0.144
0.122	0.225	0.183	-0.247	-0.153	0.266	-0.211	-0.516
0.512	0.252	-0.304	-0.097	0.353	-0.084	0.174	-0.286
0.698	0.177	-0.074	-0.126	0.161	0.013	-0.050	-0.173
1.000	0.316	0.000	-0.316	0.316	0.000	-0.316	-0.000
1.257	0.285	-0.092	-0.169	0.305	-0.214	-0.266	0.293
1.318	0.293	-0.493	0.357	0.022	-0.387	0.107	-0.053
1.370	0.024	-0.205	0.258	-0.148	-0.055	0.173	-0.228
1.765	0.073	-0.153	0.198	-0.196	0.148	0.025	-0.293
2.192	0.320	-0.269	0.268	-0.320	0.432	-0.434	0.220
2.369	0.115	-0.079	0.072	-0.092	0.145	-0.194	0.220

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.742	0.274	0.125	0.059	0.038	0.045	0.021	0.013
-2.645	0.515	0.278	0.147	0.111	0.146	0.073	0.049
-2.461	0.543	-0.066	-0.072	-0.112	-0.204	-0.118	-0.087
-2.104	0.027	-0.028	-0.138	-0.263	-0.414	-0.328	-0.275
-2.000	-0.000	-0.000	-0.000	0.000	0.000	0.000	0.000
-2.000	-0.333	0.000	-0.000	-0.000	0.000	0.000	-0.000
-1.606	0.241	-0.411	-0.463	-0.333	-0.072	0.165	0.337
-1.242	-0.225	0.270	-0.039	-0.319	-0.357	-0.315	-0.035
-1.147	-0.166	0.018	0.072	0.065	0.002	0.296	0.337
-1.075	-0.080	0.127	0.109	-0.010	-0.120	0.078	0.204
-1.000	0.000	-0.316	-0.316	0.000	0.316	-0.000	-0.316
-0.583	0.101	-0.267	0.318	0.453	-0.054	-0.394	-0.176
0.122	0.243	0.011	0.160	-0.030	-0.156	0.006	0.156
0.512	0.114	-0.138	0.059	0.108	-0.115	-0.118	0.175
0.698	0.064	0.112	0.374	-0.373	-0.114	0.428	-0.185
1.000	0.000	0.316	-0.316	-0.000	0.316	-0.000	-0.316
1.257	-0.090	-0.043	0.088	-0.068	-0.003	-0.287	0.363
1.318	0.016	-0.048	-0.078	0.150	-0.120	0.172	-0.107
1.370	0.068	0.099	0.263	-0.460	0.367	-0.173	-0.130
1.765	0.078	0.464	-0.315	0.092	0.153	-0.281	0.343
2.192	-0.052	-0.043	-0.029	0.107	-0.206	0.151	-0.125
2.369	-0.050	-0.331	0.253	-0.269	0.385	-0.236	0.175

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X	C(15)	C(16)	C(17)	C(18)	C(19)	C(20)	C(21)
-2.742	0.015	0.029	0.063	0.100	0.108	0.422	0.568
-2.645	0.055	0.097	0.202	0.290	0.360	-0.200	-0.310
-2.461	-0.096	-0.149	-0.271	-0.315	-0.546	-0.047	-0.102
-2.104	-0.251	-0.253	-0.281	0.076	0.587	-0.000	-0.002
-2.000	0.000	0.000	-0.000	-0.000	-0.000	0.000	0.624
-2.000	0.000	0.000	-0.000	-0.000	0.000	-0.000	-0.204
-1.606	0.376	0.267	0.052	-0.111	0.225	0.004	-0.009
-1.242	0.272	0.373	0.191	0.221	-0.233	0.021	-0.027
-1.147	0.090	-0.233	-0.358	-0.179	0.168	0.076	-0.089
-1.075	0.141	-0.052	-0.197	-0.039	0.034	-0.145	0.157
-1.000	-0.316	0.000	0.316	-0.000	0.000	-0.000	0.000
-0.583	0.292	0.346	-0.090	-0.345	0.195	0.035	-0.025
0.122	-0.025	-0.152	0.044	0.303	-0.114	0.368	-0.173
0.512	0.028	-0.190	0.069	0.269	-0.086	-0.538	0.214
0.698	-0.299	0.394	0.024	-0.297	0.088	-0.134	0.050
1.000	0.316	-0.000	-0.316	-0.000	0.000	-0.000	0.000
1.257	-0.170	-0.150	0.358	-0.298	0.073	0.256	-0.079
1.318	-0.031	0.148	-0.164	0.188	-0.045	0.423	-0.127
1.370	0.351	-0.351	0.130	-0.194	0.046	0.056	-0.017
1.765	-0.324	0.230	-0.081	-0.240	0.051	-0.100	0.027
2.192	0.123	-0.144	0.193	-0.074	0.014	-0.216	0.052
2.369	-0.178	0.247	-0.407	0.332	-0.061	-0.066	0.015

X	C(22)
-2.742	0.455
-2.645	-0.248
-2.461	-0.081
-2.104	-0.002
-2.000	-0.781
-2.000	-0.161
-1.606	-0.007
-1.242	-0.022
-1.147	-0.072
-1.075	0.126
-1.000	0.000
-0.583	-0.020
0.122	-0.139
0.512	0.171
0.698	0.040
1.000	0.000
1.257	-0.063
1.318	-0.102
1.370	-0.013
1.765	0.021
2.192	0.041
2.369	0.012

Energi elektron π (sebelum tehnik w)
untuk asam 1-hidroksi-2-naftoil-o-benzoat

$E = 20.0000\ \alpha + 38.0411\ \beta$

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Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.713	0.946	0.731	0.718	0.978	0.762	0.556
q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
1.779	0.713	0.565	0.624	0.766	0.695	0.711
q(15)	q(16)	q(17)	q(18)	q(19)	q(20)	q(21)
0.638	0.727	0.806	0.588	1.836	0.495	1.789
q(22)						
1.865						

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.287	0.054	0.269	0.282	0.022	0.238	0.444
f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
-0.779	0.287	0.435	0.376	0.234	0.305	0.289
f(15)	f(16)	f(17)	f(18)	f(19)	f(20)	f(21)
0.362	0.273	0.194	0.412	-1.836	0.505	-0.789
f(22)						
-1.865						

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 6)	(2 3)	(3 4)	(4 5)	(5 6)	(5 20)
0.662	0.412	0.655	0.448	0.636	0.546	0.391
(6 7)	(7 8)	(7 9)	(9 10)	(9 18)	(10 11)	(11 12)
0.419	0.544	0.397	0.504	0.418	0.466	0.577
(12 13)	(12 17)	(13 14)	(14 15)	(15 16)	(16 17)	(17 18)
0.527	0.310	0.573	0.513	0.514	0.624	0.474
(18 19)	(20 21)	(20 22)				
0.447	0.553	0.442				

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.658	0.415	0.629	0.648	0.159	0.355	0.373
Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
3.188	0.414	0.762	0.689	0.319	0.632	0.646
Fv(15)	Fv(16)	Fv(17)	Fv(18)	Fv(19)	Fv(20)	Fv(21)
0.705	0.595	0.324	0.393	2.285	0.347	3.179
Fv(22)						
2.290						

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Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.40	0.37	0.00	0.34	0.42	0.01	0.01
fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.01	0.03	0.02	0.00	0.03	0.01	0.08
fe(15)	fe(16)	fe(17)	fe(18)	fe(19)	fe(20)	fe(21)
0.04	0.01	0.08	0.00	0.00	0.04	0.05
fe(22)						
0.03						

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.20	0.00	0.20	0.20	0.00	0.20	0.00
fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.00	0.20	0.20	0.00	0.20	0.00	0.20
fn(15)	fn(16)	fn(17)	fn(18)	fn(19)	fn(20)	fn(21)
0.20	0.00	0.20	0.00	0.00	0.00	0.00
fn(22)						
0.00						

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.30	0.19	0.10	0.27	0.21	0.10	0.01
fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.01	0.12	0.11	0.00	0.11	0.01	0.14
fr(15)	fr(16)	fr(17)	fr(18)	fr(19)	fr(20)	fr(21)
0.12	0.00	0.14	0.00	0.00	0.02	0.02
fr(22)						
0.02						

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Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.53	0.73	0.52	0.53	0.71	0.48	0.27

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.82	0.43	0.34	0.40	0.45	0.48	0.50

Se(15)	Se(16)	Se(17)	Se(18)	Se(19)	Se(20)	Se(21)
0.42	0.50	0.53	0.31	0.88	0.21	0.81

Se(22)
0.88

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.50	1.47	1.49	1.26	1.68	1.22	5.09

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
1.02	0.23	0.78	0.19	0.89	0.42	0.93

Sn(15)	Sn(16)	Sn(17)	Sn(18)	Sn(19)	Sn(20)	Sn(21)
0.36	0.93	0.47	2.04	0.16	3.83	0.71

Sn(22)
0.46

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.01	1.10	1.01	0.89	1.20	0.85	2.68

Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.92	0.33	0.56	0.29	0.67	0.45	0.72

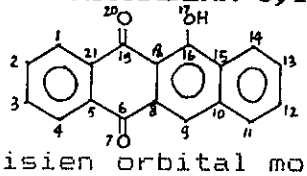
Sr(15)	Sr(16)	Sr(17)	Sr(18)	Sr(19)	Sr(20)	Sr(21)
0.39	0.72	0.50	1.18	0.52	2.02	0.76

Sr(22)
0.67

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LAMPIRAN XVIII

HASIL PERHITUNGAN UNTUK MOLEKUL 6-HIDROKSITETRASENA-5,12-KUINON



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk 6-hidroksitetrasena-5,12-kuinon

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.810	0.108	0.059	0.059	0.106	0.238	0.320	0.395
-2.542	0.016	-0.005	-0.030	-0.070	-0.149	-0.354	-0.654
-2.468	0.084	0.051	0.041	0.051	0.084	-0.000	-0.000
-2.102	0.020	0.019	0.020	0.023	0.028	0.013	0.128
-2.000	0.354	0.354	0.354	0.354	0.354	-0.000	-0.354
-1.660	0.102	0.149	0.146	0.093	0.008	-0.099	0.291
-1.259	0.056	-0.174	-0.275	-0.172	0.058	0.001	-0.002
-1.193	0.177	0.365	0.258	-0.057	-0.326	-0.178	0.221
-1.102	0.465	0.201	-0.244	-0.470	-0.274	-0.144	0.161
-1.000	0.000	-0.316	-0.316	-0.000	0.316	-0.000	0.000
-0.673	0.232	0.124	-0.148	-0.224	-0.002	0.190	-0.143
-0.085	0.198	0.201	-0.181	-0.216	0.163	0.414	-0.216
0.444	0.244	-0.151	-0.177	0.229	0.075	-0.305	0.125
0.819	0.408	-0.230	-0.219	0.410	-0.116	-0.210	0.075
1.000	0.000	0.316	-0.316	0.000	0.316	-0.000	0.000
1.232	0.289	-0.166	-0.085	0.270	-0.248	0.226	-0.070
1.324	0.078	-0.355	0.392	-0.164	-0.175	0.144	-0.043
1.563	0.212	-0.104	-0.049	0.181	-0.234	0.411	-0.115
1.792	0.246	-0.313	0.315	-0.252	0.136	0.136	-0.036
2.210	0.235	-0.195	0.195	-0.236	0.327	-0.161	0.038
2.510	0.159	-0.106	0.105	-0.159	0.293	-0.283	0.063

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.810	0.266	0.136	0.116	0.052	0.030	0.032	0.061
-2.542	-0.098	-0.022	0.043	0.025	0.021	0.029	0.053
-2.468	-0.084	-0.123	-0.220	-0.127	-0.093	-0.103	-0.160
-2.102	-0.128	-0.257	-0.412	-0.327	-0.275	-0.252	-0.254
-2.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
-1.660	-0.464	-0.296	-0.027	0.164	0.299	0.332	0.253
-1.259	-0.055	-0.331	-0.362	-0.266	0.026	0.299	0.351
-1.193	-0.108	-0.021	0.084	-0.258	-0.392	-0.209	0.142
-1.102	-0.046	0.068	0.120	0.233	0.136	-0.082	-0.227
-1.000	-0.316	-0.000	0.316	0.000	-0.316	-0.316	-0.000
-0.673	0.273	0.322	-0.056	-0.357	-0.184	0.233	0.341
-0.085	0.089	-0.361	-0.119	0.188	0.135	-0.176	-0.150
0.444	-0.064	0.364	-0.097	-0.275	0.219	0.178	-0.298
0.819	0.214	-0.165	-0.079	0.328	-0.190	-0.173	0.331
1.000	-0.316	-0.000	0.316	0.000	-0.316	0.316	0.000
1.232	0.039	-0.286	0.313	-0.344	0.111	0.208	-0.367
1.324	0.027	-0.171	0.199	0.149	-0.396	0.375	-0.101
1.563	-0.293	0.303	-0.180	0.161	-0.071	-0.050	0.148
1.792	-0.344	0.119	0.131	-0.238	0.296	-0.292	0.227
2.210	-0.009	0.165	-0.355	0.257	-0.214	0.215	-0.261
2.510	0.354	-0.244	0.260	-0.141	0.094	-0.095	0.144

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X	C(15)	C(16)	C(17)	C(18)	C(19)	C(20)	C(21)
-2.810	0.139	0.213	0.210	0.291	0.340	0.419	0.244
-2.542	0.105	0.171	0.253	0.128	0.251	0.464	0.047
-2.468	-0.293	-0.343	-0.587	-0.084	0.219	0.468	0.157
-2.102	-0.282	0.074	0.577	-0.026	0.000	0.004	0.023
-2.000	-0.000	0.000	0.000	0.000	0.000	-0.353	0.354
-1.660	0.087	-0.081	0.191	-0.375	-0.077	0.227	0.020
-1.259	0.142	0.190	-0.205	0.260	0.193	-0.261	0.244
-1.193	0.379	0.226	-0.224	0.070	-0.034	0.042	-0.153
-1.102	-0.168	-0.078	0.070	0.026	0.153	-0.170	0.312
-1.000	0.316	0.000	-0.000	-0.316	0.000	-0.000	0.316
-0.673	-0.003	-0.287	0.173	-0.328	-0.208	0.156	0.032
-0.085	0.163	0.284	-0.118	-0.045	-0.376	0.196	-0.184
0.444	-0.045	0.416	-0.136	-0.030	-0.338	0.138	0.042
0.819	-0.098	-0.171	0.049	0.200	-0.206	0.073	-0.104
1.000	-0.316	-0.000	-0.000	0.316	-0.000	0.000	-0.316
1.232	0.244	-0.247	0.061	0.012	0.194	-0.060	-0.190
1.324	-0.241	0.222	-0.053	-0.010	-0.236	0.071	0.252
1.563	-0.182	0.316	-0.071	-0.255	0.376	-0.105	-0.227
1.792	-0.116	-0.152	0.032	0.362	-0.153	0.040	-0.128
2.210	0.362	-0.184	0.035	0.017	0.157	-0.037	-0.325
2.510	-0.266	0.265	-0.047	-0.361	0.286	-0.064	-0.295

Energi elektron π (sebelum tehnik w)
untuk 6-hidroksitetrasena-9,12-kuinon

$E = 20.0000\ \alpha + 36.2713\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.811	0.915	0.908	0.812	0.993	0.581	1.770

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
0.871	0.604	0.972	0.690	0.895	0.853	0.710

q(15)	q(16)	q(17)	q(18)	q(19)	q(20)	q(21)
0.990	0.595	1.838	0.846	0.589	1.771	0.985

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.189	0.085	0.092	0.188	0.007	0.419	-0.770

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.129	0.396	0.028	0.310	0.105	0.147	0.290

f(15)	f(16)	f(17)	f(18)	f(19)	f(20)	f(21)
0.010	0.405	-1.838	0.154	0.411	-0.771	0.015

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 21)	(2 3)	(3 4)	(4 5)	(5 6)	(5 21)
0.599	0.599	0.691	0.593	0.607	0.452	0.538

(6 7)	(6 8)	(8 9)	(8 18)	(9 10)	(10 11)	(10 15)
0.537	0.380	0.472	0.652	0.564	0.536	0.518

(11 12)	(12 13)	(13 14)	(14 15)	(15 16)	(16 17)	(16 18)
0.557	0.717	0.524	0.592	0.492	0.443	0.409

(18 19)	(19 20)	(19 21)
0.387	0.533	0.455

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.534	0.442	0.448	0.532	0.135	0.363	3.195

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.228	0.696	0.115	0.639	0.458	0.492	0.616

Fv(15)	Fv(16)	Fv(17)	Fv(18)	Fv(19)	Fv(20)	Fv(21)
0.130	0.388	2.289	0.284	0.357	3.199	0.140

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.00	0.20	0.20	0.00	0.20	0.00	0.00

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.20	0.00	0.20	0.00	0.20	0.20	0.00

fe(15)	fe(16)	fe(17)	fe(18)	fe(19)	fe(20)	fe(21)
0.20	0.00	0.00	0.20	0.00	0.00	0.20

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.11	0.03	0.04	0.10	0.00	0.07	0.04

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.15	0.21	0.01	0.25	0.07	0.11	0.23

fn(15)	fn(16)	fn(17)	fn(18)	fn(19)	fn(20)	fn(21)
0.00	0.16	0.06	0.22	0.09	0.05	0.00

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.05	0.12	0.12	0.05	0.10	0.04	0.02
fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.17	0.10	0.10	0.13	0.13	0.15	0.12
fr(15)	fr(16)	fr(17)	fr(18)	fr(19)	fr(20)	fr(21)
0.10	0.08	0.03	0.21	0.04	0.02	0.10

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.60	0.70	0.69	0.60	0.71	0.27	0.82
Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.57	0.38	0.66	0.47	0.68	0.63	0.49
Se(15)	Se(16)	Se(17)	Se(18)	Se(19)	Se(20)	Se(21)
0.70	0.32	0.88	0.57	0.28	0.82	0.70

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
-0.07	-0.16	0.02	-0.26	0.04	-3.17	-1.04
Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
0.27	-2.34	0.36	-0.21	0.38	-0.05	0.19
Sn(15)	Sn(16)	Sn(17)	Sn(18)	Sn(19)	Sn(20)	Sn(21)
0.02	-0.87	-0.31	0.27	-2.40	-0.85	-0.16

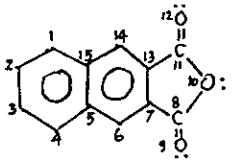
Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.27	0.27	0.36	0.17	0.37	-1.45	-0.11
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
0.42	-0.98	0.51	0.13	0.53	0.29	0.34
Sr(15)	Sr(16)	Sr(17)	Sr(18)	Sr(19)	Sr(20)	Sr(21)
0.36	-0.28	0.29	0.42	-1.06	-0.01	0.27

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LAMPIRAN XIX

HASIL PERHITUNGAN UNTUK MOLEKUL NAFTALEN-2, 3-DIKARBOKSILAT ANHIDRAT



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk naftalen-2,3-dikarboksilat anhidrad

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.962	0.025	0.013	0.013	0.025	0.062	0.098	0.228
-2.463	0.001	-0.002	-0.006	-0.012	-0.024	-0.052	-0.105
-2.288	0.300	0.233	0.233	0.300	0.453	0.282	0.193
-2.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-1.659	0.258	0.390	0.389	0.255	0.035	-0.237	-0.427
-1.326	0.371	0.150	-0.172	-0.378	-0.329	-0.400	-0.201
-1.074	0.047	0.444	0.429	0.017	-0.411	-0.065	0.341
-0.718	0.431	0.241	-0.258	-0.426	-0.048	0.323	0.280
0.098	0.129	0.165	-0.146	-0.151	0.160	0.313	-0.191
0.462	0.343	-0.230	-0.236	0.339	0.080	-0.448	0.127
1.072	0.403	-0.156	-0.236	0.409	-0.202	0.084	0.112
1.186	0.139	-0.508	0.463	-0.042	-0.414	0.190	0.189
1.445	0.226	-0.062	-0.137	0.260	-0.238	0.350	-0.268
1.855	0.294	-0.341	0.338	-0.286	0.192	0.134	-0.441
2.370	0.251	-0.184	0.184	-0.252	0.414	-0.318	0.339

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)	C(15)
-2.962	0.365	0.379	0.591	0.346	0.360	0.213	0.092	0.061
-2.463	-0.287	-0.620	0.022	0.300	0.648	0.081	0.035	0.005
-2.288	-0.039	-0.136	-0.183	-0.027	-0.094	0.198	0.285	0.454
-2.000	-0.000	0.530	-0.662	-0.000	0.530	0.000	0.000	0.000
-1.659	-0.054	0.157	0.226	-0.043	0.125	-0.418	-0.229	0.039
-1.326	-0.070	0.104	0.005	0.067	-0.099	0.204	0.412	0.342
-1.074	0.100	-0.108	-0.156	0.080	-0.087	0.331	-0.058	-0.393
-0.718	0.186	-0.145	-0.000	-0.186	0.145	-0.309	-0.334	0.069
0.098	-0.499	0.238	0.003	0.493	-0.235	0.205	-0.272	-0.178
0.462	0.250	-0.102	-0.177	0.293	-0.119	0.139	-0.455	0.072
1.072	-0.378	0.123	0.212	-0.437	0.142	0.174	0.095	-0.276
1.186	-0.227	0.071	0.011	0.182	-0.057	-0.187	-0.132	0.343
1.445	0.343	-0.100	-0.161	0.350	-0.102	-0.307	0.396	-0.265
1.855	0.283	-0.073	-0.013	-0.220	0.057	0.401	-0.106	-0.205
2.370	-0.160	0.037	0.005	0.135	-0.031	-0.325	0.311	-0.412

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Energi elektron π (sebelum tehnik w)
untuk naftalen-2,3-dikarboksilat anhidrad

E = 16.0000 α +28.9782 β

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.967	0.968	0.973	0.961	0.980	0.834	1.035

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
0.539	1.792	1.795	0.515	1.785	1.025	0.856

q(15)
0.975

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.033	0.032	0.027	0.039	0.020	0.166	-0.035

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.461	-0.792	0.205	0.485	-0.785	-0.025	0.144

f(15)
0.025

Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 15)	(2 3)	(3 4)	(4 5)	(5 6)	(5 15)
0.703	0.572	0.617	0.704	0.568	0.540	0.512

(6 7)	(7 8)	(7 13)	(8 9)	(8 10)	(10 11)	(11 12)
0.664	0.458	0.485	0.536	0.376	0.389	0.551

(11 13)	(13 14)	(14 15)
0.416	0.685	0.534

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.458	0.412	0.411	0.460	0.111	0.527	0.124

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.361	3.196	1.967	0.376	3.181	0.145	0.513

Fv(15)
0.115

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Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.37	0.12	0.13	0.36	0.00	0.21	0.16

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.07	0.04	0.00	0.07	0.04	0.19	0.22

fe(15)
0.01

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.03	0.05	0.04	0.05	0.05	0.20	0.07

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.50	0.11	0.00	0.49	0.11	0.08	0.15

fn(15)
0.06

Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.20	0.09	0.09	0.20	0.03	0.20	0.11

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.28	0.08	0.00	0.28	0.08	0.14	0.19

fr(15)
0.04

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.89	0.79	0.80	0.88	0.67	0.69	0.79

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.28	0.83	0.81	0.27	0.82	0.81	0.71

Se(15)
0.66

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Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
1.40	1.43	1.32	1.51	1.18	3.22	1.30

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
5.98	1.26	0.26	5.97	1.25	1.45	2.76

Sn(15)
1.29

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
1.15	1.11	1.06	1.20	0.92	1.95	1.05

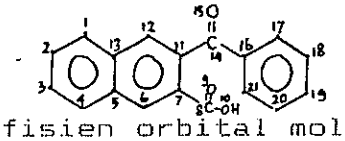
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
3.13	1.05	0.53	3.12	1.03	1.13	1.74

Sr(15)
0.98

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LAMPIRAN XX

HASIL PERHITUNGAN UNTUK MOLEKUL ASAM-2-BENZOIL-o-KARBOKSILAT



Hasil perhitungan koefisien orbital molekul Huckel
(sebelum tehnik w) untuk asam 2-benzoil-o-karboksilat

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.743	0.039	0.023	0.024	0.043	0.093	0.128	0.258
-2.597	0.037	0.021	0.018	0.026	0.050	0.030	0.029
-2.278	0.296	0.232	0.232	0.297	0.444	0.272	0.175
-2.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-2.000	0.000	0.000	0.000	0.000	-0.000	-0.000	-0.000
-1.675	0.251	0.375	0.377	0.256	0.052	-0.215	-0.412
-1.325	0.381	0.195	-0.123	-0.358	-0.351	-0.417	-0.201
-1.161	0.056	-0.256	-0.353	-0.154	0.175	0.036	-0.133
-1.033	0.076	0.358	0.293	-0.055	-0.350	-0.027	0.322
-1.000	0.000	0.001	0.001	-0.000	-0.001	0.000	0.001
-0.680	0.423	0.248	-0.255	-0.421	-0.031	0.359	0.276
0.140	0.161	0.082	-0.173	-0.058	0.181	0.137	-0.200
0.386	0.230	-0.254	-0.132	0.305	0.014	-0.475	0.169
0.809	0.349	-0.086	-0.280	0.312	0.027	-0.137	0.084
1.000	0.000	0.000	-0.000	-0.000	-0.000	-0.000	-0.000
1.134	0.289	-0.444	0.215	0.200	-0.442	0.185	0.232
1.262	0.126	0.250	-0.442	0.307	0.054	0.034	-0.097
1.429	0.258	-0.164	-0.024	0.199	-0.259	0.378	-0.280
1.828	0.265	-0.316	0.313	-0.256	0.155	0.140	-0.412
2.118	0.142	-0.131	0.135	-0.154	0.192	-0.082	-0.019
2.383	0.236	-0.170	0.170	-0.235	0.389	-0.300	0.326

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.743	0.435	0.586	0.469	0.188	0.100	0.085	0.177
-2.597	-0.171	-0.286	-0.229	0.198	0.105	0.074	0.423
-2.278	-0.043	-0.157	-0.125	0.167	0.267	0.442	-0.070
-2.000	-0.000	0.625	-0.781	0.000	0.000	0.000	-0.000
-2.000	-0.000	0.000	0.000	-0.000	-0.000	-0.000	0.000
-1.675	-0.055	0.170	0.136	-0.426	-0.227	0.046	-0.083
-1.325	-0.048	0.072	0.057	0.194	0.380	0.310	0.087
-1.161	-0.039	0.046	0.037	-0.156	0.142	0.321	-0.210
-1.033	0.106	-0.110	-0.088	0.264	-0.014	-0.279	-0.038
-1.000	0.000	-0.000	-0.000	0.001	-0.000	-0.001	-0.000
-0.680	0.129	-0.098	-0.078	-0.288	-0.364	0.040	-0.119
0.140	-0.288	0.134	0.107	0.150	-0.328	-0.104	0.563
0.386	0.506	-0.212	-0.170	-0.046	-0.308	0.165	0.173
0.809	-0.337	0.120	0.096	0.372	-0.217	-0.197	-0.187
1.000	0.000	0.000	0.000	0.000	0.000	-0.000	-0.000
1.134	-0.343	0.109	0.087	-0.140	0.021	0.116	-0.105
1.262	0.115	-0.035	-0.028	-0.015	0.336	-0.410	-0.245
1.429	0.265	-0.077	-0.062	-0.216	0.295	-0.205	0.327
1.828	0.265	-0.069	-0.055	0.375	-0.113	-0.168	-0.178
2.118	0.010	-0.002	-0.002	0.113	0.027	-0.171	-0.275
2.383	-0.146	0.033	0.027	-0.345	0.309	-0.392	0.208

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X	C(15)	C(16)	C(17)	C(18)	C(19)	C(20)	C(21)
-2.743	0.238	0.086	0.038	0.019	0.014	0.019	0.038
-2.597	0.709	0.235	0.115	0.063	0.048	0.063	0.115
-2.278	-0.253	-0.063	-0.040	-0.029	-0.025	-0.029	-0.040
-2.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
-2.000	0.345	-0.383	-0.383	-0.383	-0.383	-0.383	-0.383
-1.675	0.255	-0.011	0.028	0.058	0.069	0.058	0.028
-1.325	-0.128	0.076	0.011	-0.061	-0.092	-0.061	0.011
-1.161	0.251	-0.394	-0.134	0.239	0.411	0.239	-0.134
-1.033	0.040	-0.352	-0.163	0.183	0.353	0.181	-0.166
-1.000	-0.000	-0.001	-0.500	-0.500	0.001	0.500	0.500
-0.680	0.090	0.097	0.087	-0.038	-0.113	-0.038	0.087
0.140	-0.263	0.054	-0.257	-0.018	0.260	-0.018	-0.257
0.386	-0.073	0.052	-0.088	-0.018	0.095	-0.018	-0.088
0.809	0.067	-0.278	0.197	0.118	-0.293	0.118	0.197
1.000	0.000	0.000	-0.500	0.500	0.000	-0.500	0.500
1.134	0.033	0.235	-0.086	-0.137	0.242	-0.137	-0.086
1.262	0.075	0.275	-0.063	-0.196	0.310	-0.195	-0.063
1.429	-0.095	-0.197	-0.006	0.206	-0.288	0.206	-0.006
1.828	0.046	-0.065	0.140	-0.190	0.208	-0.190	0.140
2.118	0.067	0.460	-0.364	0.310	-0.293	0.310	-0.364
2.383	-0.047	-0.152	0.088	-0.057	0.048	-0.057	0.088

Energi elektron π (sebelum tehnik w)
untuk asam 1-benzoil-o-karboksilat

$E = 20.0000\ \alpha + 35.6201\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.616	0.854	0.845	0.622	0.975	0.627	0.859

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
0.477	1.776	1.857	0.831	0.617	0.974	0.551

q(15)	q(16)	q(17)	q(18)	q(19)	q(20)	q(21)
1.776	0.997	0.918	0.998	0.913	0.998	0.918

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.384	0.146	0.155	0.378	0.025	0.373	0.141

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.523	-0.776	-1.857	0.169	0.383	0.026	0.449

f(15)	f(16)	f(17)	f(18)	f(19)	f(20)	f(21)
-0.776	0.003	0.082	0.002	0.087	0.002	0.082

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Urdo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 13)	(2 3)	(3 4)	(4 5)	(5 6)	(5 13)
0.504	0.526	0.735	0.498	0.537	0.571	0.510

(6 7)	(7 8)	(7 11)	(8 9)	(8 10)	(11 12)	(11 14)
0.481	0.343	0.651	0.569	0.455	0.457	0.360

(12 13)	(14 15)	(14 16)	(16 17)	(16 21)	(17 18)	(18 19)
0.583	0.547	0.446	0.582	0.582	0.690	0.645

(19 20)	(20 21)
0.645	0.690

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.701	0.493	0.499	0.697	0.114	0.680	0.257

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.366	3.163	2.277	0.264	0.693	0.113	0.379

Fv(15)	Fv(16)	Fv(17)	Fv(18)	Fv(19)	Fv(20)	Fv(21)
3.185	0.122	0.460	0.397	0.441	0.397	0.460

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.00	0.00	0.00	0.00	0.00	0.00	0.00

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.00	0.00	0.00	0.00	0.00	0.00	0.00

fe(15)	fe(16)	fe(17)	fe(18)	fe(19)	fe(20)	fe(21)
0.00	0.00	0.50	0.50	0.00	0.50	0.50

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.36	0.12	0.13	0.35	0.00	0.26	0.15

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.03	0.02	0.01	0.17	0.27	0.00	0.03

fn(15)	fn(16)	fn(17)	fn(18)	fn(19)	fn(20)	fn(21)
0.02	0.02	0.02	0.00	0.03	0.00	0.02

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.18	0.06	0.06	0.18	0.00	0.13	0.08
fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.02	0.01	0.01	0.08	0.13	0.00	0.01
fr(15)	fr(16)	fr(17)	fr(18)	fr(19)	fr(20)	fr(21)
0.01	0.01	0.26	0.25	0.01	0.25	0.26

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.39	0.63	0.62	0.40	0.66	0.40	0.57
Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.19	0.79	0.87	0.53	0.39	0.66	0.26
Se(15)	Se(16)	Se(17)	Se(18)	Se(19)	Se(20)	Se(21)
0.82	0.71	0.74	0.82	0.70	0.82	0.74

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.83	0.90	1.06	0.66	1.10	1.47	1.01
Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
3.16	0.54	0.34	0.80	2.14	0.92	5.13
Sn(15)	Sn(16)	Sn(17)	Sn(18)	Sn(19)	Sn(20)	Sn(21)
1.03	0.71	1.73	0.82	1.68	0.82	1.73

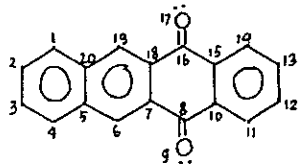
Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.61	0.77	0.84	0.53	0.88	0.93	0.79
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
1.68	0.67	0.61	0.66	1.27	0.79	2.70
Sr(15)	Sr(16)	Sr(17)	Sr(18)	Sr(19)	Sr(20)	Sr(21)
0.93	0.71	1.24	0.82	1.19	0.82	1.24

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LAMPIRAN XXI

HASIL PERHITUNGAN UNTUK MOLEKUL TETRASENA-5,12-KUINON



Hasil perhitungan koefisien orbital molekul Huckel (sebelum tehnik w) untuk tetrasena-5,12-kuinon

X	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
-2.788	0.044	0.025	0.025	0.044	0.098	0.131	0.267
-2.531	0.007	0.002	-0.002	-0.007	-0.015	-0.048	-0.105
-2.275	0.298	0.234	0.234	0.298	0.445	0.269	0.167
-2.000	0.000	-0.000	0.000	-0.000	-0.000	0.000	0.000
-1.693	0.248	0.358	0.358	0.248	0.061	-0.205	-0.409
-1.341	0.348	0.148	-0.149	-0.348	-0.318	-0.397	-0.214
-1.221	0.074	0.337	0.337	0.074	-0.246	-0.129	0.089
-1.106	0.179	0.085	-0.085	-0.179	-0.113	-0.059	0.048
-1.000	0.000	-0.316	-0.316	-0.000	0.316	0.000	-0.316
-0.717	0.403	0.235	-0.235	-0.403	-0.055	0.310	0.277
-0.115	0.164	0.147	-0.147	-0.164	0.128	0.307	-0.093
0.398	0.288	-0.206	-0.206	0.288	0.091	-0.415	0.074
0.813	0.307	-0.169	-0.169	0.307	-0.080	-0.162	0.212
1.000	0.000	-0.316	0.316	-0.000	-0.316	-0.000	0.316
1.219	0.379	-0.171	-0.171	0.379	-0.291	0.267	-0.035
1.316	0.124	-0.392	0.392	-0.124	-0.229	0.196	-0.029
1.546	0.148	-0.058	-0.058	0.148	-0.171	0.287	-0.273
1.789	0.227	-0.288	0.288	-0.227	0.118	0.134	-0.357
2.205	0.266	-0.221	0.221	-0.266	0.366	-0.175	0.019
2.500	0.140	-0.093	0.093	-0.140	0.257	-0.245	0.356

X	C(8)	C(9)	C(10)	C(11)	C(12)	C(13)	C(14)
-2.788	0.347	0.441	0.259	0.116	0.065	0.065	0.116
-2.531	-0.323	-0.607	-0.105	-0.047	-0.013	0.013	0.047
-2.275	-0.056	-0.202	-0.092	-0.062	-0.048	-0.048	-0.062
-2.000	-0.000	-0.354	0.354	0.354	0.354	0.354	0.354
-1.693	-0.078	0.253	0.023	0.094	0.136	0.136	0.094
-1.341	-0.104	0.158	-0.083	-0.091	-0.039	0.039	0.091
-1.221	0.148	-0.191	0.283	-0.086	-0.388	-0.388	-0.086
-1.106	0.160	-0.179	0.307	0.487	0.232	-0.231	-0.487
-1.000	0.000	-0.000	0.317	0.001	-0.316	-0.316	-0.000
-0.717	0.165	-0.129	-0.029	-0.215	-0.125	0.125	0.215
-0.115	-0.411	0.218	-0.172	0.219	0.197	-0.197	-0.219
0.398	0.311	-0.130	-0.068	-0.216	0.154	0.154	-0.216
0.813	-0.222	0.079	-0.110	0.422	-0.233	-0.233	0.422
1.000	0.000	-0.000	-0.316	-0.000	0.316	-0.316	0.000
1.219	-0.190	0.059	0.207	-0.270	0.122	0.122	-0.270
1.316	-0.187	0.056	0.218	0.118	-0.374	0.374	-0.118
1.546	0.407	-0.115	-0.243	0.210	-0.083	-0.083	0.210
1.789	0.148	-0.039	0.131	-0.252	0.319	-0.319	0.252
2.205	0.152	-0.036	-0.317	0.231	-0.192	0.192	-0.231
2.500	-0.289	0.064	0.303	-0.165	0.110	-0.110	0.165

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X	C(15)	C(16)	C(17)	C(18)	C(19)	C(20)
-2.788	0.259	0.347	0.440	0.267	0.131	0.098
-2.531	0.105	0.323	0.608	0.105	0.048	0.015
-2.275	-0.092	-0.056	-0.202	0.167	0.269	0.445
-2.000	0.353	-0.000	-0.354	0.000	0.000	-0.000
-1.693	0.023	-0.078	0.253	-0.408	-0.205	0.062
-1.341	0.083	0.104	-0.158	0.214	0.397	0.318
-1.221	0.283	0.148	-0.191	0.089	-0.129	-0.246
-1.106	-0.307	-0.160	0.179	-0.048	0.059	0.113
-1.000	0.316	-0.000	0.000	-0.316	-0.000	0.316
-0.717	0.029	-0.165	0.129	-0.277	-0.310	0.054
-0.115	0.172	0.411	-0.218	0.093	-0.307	-0.128
0.398	-0.068	0.311	-0.130	0.074	-0.415	0.091
0.813	-0.110	-0.222	0.079	0.212	-0.162	-0.080
1.000	0.316	-0.000	0.000	-0.316	-0.000	0.316
1.219	0.207	-0.190	0.059	-0.035	0.267	-0.291
1.316	-0.218	0.187	-0.056	0.029	-0.196	0.229
1.546	-0.243	0.407	-0.115	-0.273	0.287	-0.171
1.789	-0.131	-0.148	0.039	0.357	-0.134	-0.118
2.205	0.317	-0.152	0.036	-0.019	0.175	-0.366
2.500	-0.303	0.289	-0.064	-0.356	0.245	-0.257

Energi elektron π^2 (sebelum tehnik w)
untuk tetrasena- 5,12- Kuinon

$E = 20.0000\ \alpha + 33.3436\ \beta$

Kerapatan elektron (sebelum tehnik w)

q(1)	q(2)	q(3)	q(4)	q(5)	q(6)	q(7)
0.947	0.962	0.962	0.947	0.977	0.814	1.019

q(8)	q(9)	q(10)	q(11)	q(12)	q(13)	q(14)
0.639	1.805	0.989	0.905	0.943	0.943	0.905

q(15)	q(16)	q(17)	q(18)	q(19)	q(20)
0.989	0.639	1.805	1.019	0.814	0.977

Muatan neto (sebelum tehnik w)

f(1)	f(2)	f(3)	f(4)	f(5)	f(6)	f(7)
0.053	0.038	0.038	0.053	0.023	0.186	-0.019

f(8)	f(9)	f(10)	f(11)	f(12)	f(13)	f(14)
0.361	-0.805	0.011	0.095	0.057	0.057	0.095

f(15)	f(16)	f(17)	f(18)	f(19)	f(20)
0.011	0.361	-0.805	-0.019	0.186	0.023

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Ordo ikatan elektron π (sebelum tehnik w)

(1 2)	(1 20)	(2 3)	(3 4)	(4 5)	(5 6)	(5 20)
0.692	0.574	0.624	0.692	0.574	0.536	0.509

(6 7)	(7 8)	(7 18)	(8 9)	(8 10)	(10 11)	(10 15)
0.650	0.476	0.477	0.492	0.444	0.614	0.536

(11 12)	(12 13)	(13 14)	(14 15)	(15 16)	(16 17)	(16 18)
0.651	0.659	0.651	0.614	0.444	0.492	0.476

(18 19)	(19 20)
0.650	0.536

Free valensi (sebelum tehnik w)

Fv(1)	Fv(2)	Fv(3)	Fv(4)	Fv(5)	Fv(6)	Fv(7)
0.466	0.416	0.416	0.466	0.113	0.546	0.129

Fv(8)	Fv(9)	Fv(10)	Fv(11)	Fv(12)	Fv(13)	Fv(14)
0.321	3.240	0.138	0.467	0.422	0.422	0.467

Fv(15)	Fv(16)	Fv(17)	Fv(18)	Fv(19)	Fv(20)
0.138	0.321	3.240	0.129	0.546	0.113

Indeks kereaktifan (frontier orbital) terhadap elektrofil (sebelum tehnik w)

fe(1)	fe(2)	fe(3)	fe(4)	fe(5)	fe(6)	fe(7)
0.33	0.11	0.11	0.33	0.01	0.19	0.15

fe(8)	fe(9)	fe(10)	fe(11)	fe(12)	fe(13)	fe(14)
0.05	0.03	0.00	0.09	0.03	0.03	0.09

fe(15)	fe(16)	fe(17)	fe(18)	fe(19)	fe(20)
0.00	0.05	0.03	0.15	0.19	0.01

Indeks kereaktifan (frontier orbital) terhadap nukleofil (sebelum tehnik w)

fn(1)	fn(2)	fn(3)	fn(4)	fn(5)	fn(6)	fn(7)
0.05	0.04	0.04	0.05	0.03	0.19	0.02

fn(8)	fn(9)	fn(10)	fn(11)	fn(12)	fn(13)	fn(14)
0.34	0.09	0.06	0.10	0.08	0.08	0.10

fn(15)	fn(16)	fn(17)	fn(18)	fn(19)	fn(20)
0.06	0.34	0.09	0.02	0.19	0.03

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Indeks kereaktifan (frontier orbital) terhadap radikal (sebelum tehnik w)

fr(1)	fr(2)	fr(3)	fr(4)	fr(5)	fr(6)	fr(7)
0.19	0.08	0.08	0.19	0.02	0.19	0.09

fr(8)	fr(9)	fr(10)	fr(11)	fr(12)	fr(13)	fr(14)
0.20	0.06	0.03	0.09	0.05	0.05	0.09

fr(15)	fr(16)	fr(17)	fr(18)	fr(19)	fr(20)
0.03	0.20	0.06	0.09	0.19	0.02

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap elektrofil (sebelum tehnik w)

Se(1)	Se(2)	Se(3)	Se(4)	Se(5)	Se(6)	Se(7)
0.85	0.79	0.79	0.85	0.67	0.66	0.78

Se(8)	Se(9)	Se(10)	Se(11)	Se(12)	Se(13)	Se(14)
0.35	0.87	0.70	0.73	0.74	0.74	0.73

Se(15)	Se(16)	Se(17)	Se(18)	Se(19)	Se(20)
0.70	0.35	0.87	0.78	0.66	0.67

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap nukleofil (sebelum tehnik w)

Sn(1)	Sn(2)	Sn(3)	Sn(4)	Sn(5)	Sn(6)	Sn(7)
0.60	0.54	0.54	0.60	0.42	-0.34	0.53

Sn(8)	Sn(9)	Sn(10)	Sn(11)	Sn(12)	Sn(13)	Sn(14)
-1.90	-0.69	0.14	0.17	0.18	0.18	0.17

Sn(15)	Sn(16)	Sn(17)	Sn(18)	Sn(19)	Sn(20)
0.14	-1.90	-0.69	0.53	-0.34	0.42

Indeks kereaktifan (kemampuan superdelokalisasi) terhadap radikal (sebelum tehnik w)

Sr(1)	Sr(2)	Sr(3)	Sr(4)	Sr(5)	Sr(6)	Sr(7)
0.73	0.66	0.66	0.73	0.54	0.16	0.66

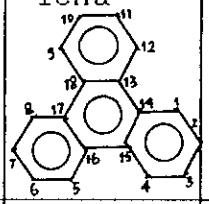
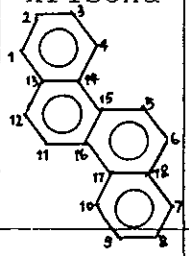
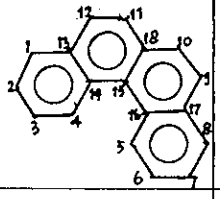
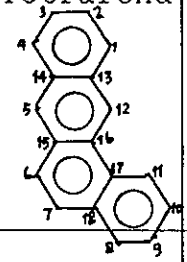
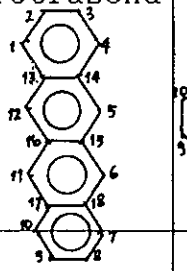
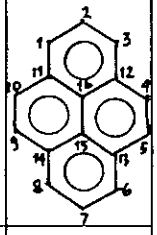
Sr(8)	Sr(9)	Sr(10)	Sr(11)	Sr(12)	Sr(13)	Sr(14)
-0.77	0.09	0.42	0.45	0.46	0.46	0.45

Sr(15)	Sr(16)	Sr(17)	Sr(18)	Sr(19)	Sr(20)
0.42	-0.77	0.09	0.66	0.16	0.54

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LAMPIRAN XXII

VALENSI BEBAS (F_r), ENERGI ELEKTRON-Π (E_π) DAN ENERGI DELOKALISASI (DE) UNTUK HIDROKARBON AROMATIK BERCINCIN EMPAT

F_r	Trifeni-lena 	Krisena 	3,4-benz-fenantrena 	Tetrafena 	Tetrasena 	Pirena 
1	0,439	0,451	0,450	0,457	0,461	0,468
2	0,405	0,403	0,404	0,408	0,410	0,393
3	0,405	0,408	0,407	0,407	0,410	0,468
4	0,439	0,442	0,445	0,458	0,461	0,452
5	0,439	0,440	0,445	0,514	0,529	0,452
6	0,405	0,457	0,407	0,455	0,529	0,468
7	0,405	0,451	0,404	0,455	0,461	0,393
8	0,439	0,403	0,450	0,450	0,410	0,468
9	0,439	0,408	0,451	0,403	0,410	0,452
10	0,405	0,442	0,448	0,409	0,461	0,452
11	0,405	0,440	0,449	0,440	0,529	0,111
12	0,439	0,457	0,451	0,502	0,529	0,111
13	0,140	0,107	0,110	0,108	0,108	0,111
14	0,140	0,138	0,132	0,105	0,108	0,111
15	0,140	0,145	0,180	0,111	0,105	0,149
16	0,140	0,145	0,132	0,140	0,105	0,149
17	0,140	0,138	0,110	0,142	0,108	-
18	0,140	0,107	0,113	0,111	0,108	-
E_π	$18\alpha + 25,2745\beta$	$18\alpha + 25,1922\beta$	$18\alpha + 25,1875\beta$	$18\alpha + 25,1012\beta$	$18\alpha + 24,9308\beta$	$16\alpha + 22,51\beta$
DE	$7,2745\beta$	$7,1922\beta$	$7,1875\beta$	$7,101\beta$	$6,9308\beta$	$6,506$

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LAMPIRAN XXIII

SIMBOL DAN MAKNANYA

AH	hidrokarbon alternant
c_{jr}	koefisien orbital atom ke-r pada orbital molekul ke-j
DE	energi delokalisasi
E_π	energi elektron-π
F_r	valensi bebas pada posisi ke-r
h_r	integral Coulomb tambahan pada orbital atom ke-r dengan satuan β_o
H_{rs}	integral Hamiltonian antara orbital r dan s
$\mathscr{H}$	matriks Hermitian
H	operator Hamiltonian
HMO	Hückel Molecular Orbital / Orbital Molekul Hückel
i,j	indeks orbital molekul
k	konstanta laju
k_{rs}	integral resonansi untuk ikatan r-s dengan satuan β_o
LCAO	kombinasi linier orbital atom
MO	orbital molekul
p_{rs}	order ikatan antara atom r-s
q_r	kerapatan elektron pada atom r
r,s	indeks atom atau orbital atom
S	integral overlap
S_r	superdelokalisabilitas pada posisi r
S_{rs}	integral overlap antara orbital atom r dan s
x	elemen diagonal dalam determinan HMO, ekivalen dengan $(\alpha-E)/\beta$

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α integral Coulomb

α_r integral Coulomb pada atom atau orbital atom ke-r

β integral resonansi

β_o integral resonansi standard

β_{rs} integral resonansi antara orbital atom r dan s

ε_i energi OM ke-i

σ_r konstanta reaktifitas substituen pada posisi r

ψ fungsi gelombang, orbital molekul

Ψ produk total fungsi gelombang

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LAMPIRAN XXIV
PROGRAM TURBO BASIC .

Sub program metode Yacobi yang ditulis dalam bahasa TURBO BASIC adalah sebagai berikut:

```
SUB Yacobi (N,A(2),R(2))
LOCAL K,L,AMAX,SIGN,AVG,R,X,Y,Z,CO,SI,B,kontrolloop,konter
'......Subrutin ini menggunakan metode Yacobi guna
'       mendiagonalkan matrik simetrik, sehingga akan didapat
'       seluruh nilai eigen dan "eigen vector" matrik.
'......Proses iterasi stop apabila elemen "off diagonal"
'       terbesar lebih kecil dari 0,0001 kali nilai rata-rata
'       elemen diagonal
'       Parameter yang dipakai:
'       N = jumlah baris/kolom dalam matrik
'       A = matrik dengan dimensi (N+1, N+1), awalnya sebagai
'           matrik masukan
'       R = array kerja yang berordo sama dengan matrik A,
'           diawali sebagai matrik identitas
'       Setelah perhitungan akan diperoleh nilai eigen sebagai
'       elemen diagonal matrik A, dan "eigen vector" pada
'       kolom-kolom matrik R.
CLS
kontrolloop = 0
konter = 0
LOCATE 1,10 : PRINT "TUNGGU SEDANG DIHITUNG"
'..Membuat matrik identitas
```

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```
FOR I = 1 TO N
  FOR J = 1 TO N
    IF I <> J THEN
       R(I,J) = 0
    END IF
  NEXT J
  R(I,I) = 1
NEXT I
DO
  konter = konter + 1
  LOCATE 3,20 : PRINT konter
  '....Mendapatkan elemen "off diagonal" terbesar
  AMAX = ABS(A(1,2))
  K = 1
  L = 2
  FOR R = 1 TO N-1
    FOR T = R+1 TO N
      IF ABS(A(R,T)) > AMAX THEN
        K = R
        L = T
        AMAX = ABS(A(R,T))
      END IF
  NEXT T
NEXT R
'..Mendapatkan harga rata-rata elemen diagonal
SUM = 0
```

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```
FOR I = 1 TO N
  SUM = SUM + ABS(A(I,I))
NEXT I
PRINT
AVG = SUM/N
'Menghitung matrik nilai eigen dan matrik eigen vector dan
'mengontrol program stop bila sarat sudah terpenuhi.
IF AMAX >= 0.0001*AVG THEN
  '..Mentransformasi elemen off diagonal menjadi nol
  '..CO = cos x    SI = sin x
  '..Dapatkan nilai sin x dan cos x
    X = 2*A(K,L)
    Y = A(K,K) - A(L,L)
    IF Y <> 0 THEN
      SIGN = (X/Y)/ABS(X/Y)
    ELSE
      SIGN = 1
    END IF
    Z = SQR(X*X + Y*Y)
    CO = SQR((Z+Y)/(2*Z))
    SI = SIGN*SQR((Z-Y)/(2*Z))
'..Menghitung matrik A_k = ..O_2^-1 O_1^-1 A  O_1 O_2..
'  (diagonalisasi matrik), tempat nilai eigen
  FOR I = 1 TO N
    IF I <> K THEN
      IF I <> L THEN
```

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```
            B = A(I,K)*CO + A(I,L)*SI
            A(I,L) = -A(I,K)*SI + A(I,L)*CO
            A(L,I) = A(I,L)
            A(I,K) = B
            A(K,I) = B
          END IF
        END IF
      NEXT I
B1 = A(K,K)*CO*CO + 2*A(K,L)*CO*SI + A(L,L)*SI*SI
Z1 = (A(L,L) - A(K,K))*CO*SI + A(K,L)*(CO*CO - SI*SI)
A(L,L) = A(K,K)*SI*SI - 2*A(K,L)*CO*SI + A(L,L)*CO*CO
       A(K,K) = B1
       A(K,L) = Z1
       A(L,K) = Z1
       '.Menghitung elemen matrik R_k = O_1 O_2 O_3 O_4 ...
       ' tempat "eigen vector"
          FOR I = 1 TO N
             B2 = R(I,K)*CO + R(I,L)*SI
             R(I,L) = -R(I,K)*SI +R(I,L)*CO
             R(I,K) = B2
           NEXT I
  ELSE
    kontrolloop = %benar
  END IF
LOOP UNTIL kontrolloop = %benar
END SUB
```

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