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ISOMERIC ADDUCT STABILITY IN THE ADDITION OF ATOMIC RADICALS TO TOLUENE: H, O(^{3}P), F and Cl.

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Supplementary Material

	H			O(^{3}P)		
	PMP2	B3LYP	BHandHLYP	PMP2	B3LYP	BHandHLYP
Ipso	-271.220127 (0.14855)	-272.1212219 (0.144582)	-271.9476105 (0.148981)	**-345.5780561** (0.140363)	-346.6668529 (0.136488)	-346.4668867 (0.140902)
Ortho	**-271.2242713** (0.148105)	**-272.1275871** (0.144218)	**-271.9533854** (0.148636)	-345.5779794 (0.140183)	**-346.6697202** (0.136061)	**-346.4693956** (0.140716)
Meta	-271.2218884 (0.14804)	-272.1252114 (0.144107)	-271.9511427 (0.148506)	-345.5750271 (0.140023)	-346.6666439 (0.13593)	-346.466656 (0.140518)
Para	-271.2219124 (0.148249)	-272.1255144 (0.144162)	-271.9512071 (0.147644)	-345.5752522 (0.140299)	-346.6674146 (0.136011)	-346.4606832 (0.142784)

	F			Cl		
	PMP2	B3LYP	BHandHLYP	PMP2	B3LYP	BHandHLYP
Ipso	**-370.2347594** (0.140803)	-371.3551097 (0.137242)	-371.1505074 (0.141434)	-730.2507045 (0.140199)	– –	-731.5375752 (0.14061)
Ortho	-370.2334128 (0.141348)	**-371.356305** (0.137739)	**-371.1511036** (0.14203)	**-730.2515029** (0.140621)	– –	**-731.5412426** (0.140983)
Meta	-370.2300954 (0.141228)	-371.3529936 (0.137608)	-371.1480249 (0.141863)	-730.2487756 (0.140475)	– –	-731.5390795 (0.140828)
Para	-370.230514 (0.141546)	-371.3540122 (0.137724)	-371.1486118 (0.142000)	-730.2493103 (0.14076)	– –	-731.5399544 (0.140944)

Electronic energies and thermal corrections of the enthalpy (TCH), in hartrees, calculated at the PMP2, B3LYP and BHandHLYP levels using the 6-31G** basis set, for the toluene + X addition reaction (X=H, O(^{3}P), F and Cl). TCH corrections are written in parenthesis. For each system and method, the lowest energy isomer has been indicated in bold face.

	Ipso		Ortho		Meta		Para	
Atom	S^2	projected	S^2	projected	S^2	projected	S^2	projected
H	1.15	0.85	1.14	0.85	1.14	0.85	1.15	0.85
O(^{3}P)	2.42	2.08	2.41	2.08	2.41	2.08	2.40	2.07
F	1.15	0.85	1.14	0.85	1.14	0.85	1.14	0.85
Cl	1.15	0.85	1.15	0.86	1.15	0.86	1.15	0.86

MP2 $< S^2 >$ values before and after spin projection for the X-toluene adducts (X = H, O(^{3}P), F and Cl).

	H			$O(^3P)$		
	MP2	B3LYP	BHandHLYP	MP2	B3LYP	BHandHLYP
Ipso	88.6	86.1	89.0	83.0	80.5	83.41
Ortho	88.2	85.8	88.6	82.8	80.2	83.2
Meta	88.1	85.6	88.5	82.7	80.0	83.0
Para	88.1	85.5	88.4	83.8	79.9	84.4
	F			Cl		
	MP2	B3LYP	BHandHLYP	MP2	B3LYP	BHandHLYP
Ipso	83.3	81.0	83.8	82.8	–	82.9
Ortho	83.5	81.2	84.0	82.9	–	83.0
Meta	83.4	81.1	83.9	82.7	–	82.9
Para	83.4	81.0	83.8	82.8	–	82.8

Zero point corrections, in kcal/mol, calculated at the MP2, B3LYP and BHandHLYP levels using the 6-31G** basis set, for the X-toluene adducts (X=H, $O(^3P)$, F and Cl).

	MP2				B3LYP				BHandHLYP			
	Ipso	Ortho	Meta	Para	Ipso	Ortho	Meta	Para	Ipso	Ortho	Meta	Para
H	80.02	80.59	81.14	83.44	80.30	80.75	81.46	86.62	79.64	80.18	80.82	77.99
$O(^3P)$	84.39	85.58	86.18	89.70	85.03	86.05	86.85	92.71	84.04	85.21	85.92	88.82
F	83.94	85.27	85.91	88.52	84.35	85.67	86.42	89.45	83.47	84.79	85.53	89.38
Cl	86.08	87.53	88.34	89.96	–	–	–	–	86.46	88.57	89.07	91.07

Entropy values S_{298}, in cal $mol^{-1}K^{-1}$ for the X-toluene adducts (X = H, $O(^3P)$, F and Cl).

Position	Atom	H	O	F	Cl
Ipso	C_1	-0.0575	-0.0624	-0.0050	-0.0497
	C_2	0.4218	0.4067	0.4038	0.3947
	C_4	0.5420	0.5555	0.5254	0.5108
	C_7	0.0568	0.1077	0.0320	0.0135
	H_9	0.0096	0.0091	0.0078	0.0084
	H_{13}	0.0002	0.0001	0.0039	0.0031
	H_{14}	-0.0019	0.0148	-0.0002	0.0013
	H_{15}	0.0002	0.0001	0.0038	0.0031
	X_{16}	0.0544	0.9684	0.0261	0.1681
Ortho	C_1	0.3958	0.4088	0.3813	0.3640
	C_2	-0.0694	-0.0508	0.0213	-0.0440
	C_3	0.4238	0.4258	0.3882	0.3653
	C_5	0.5380	0.5244	0.5135	0.4751
	C_7	-0.0292	-0.0277	-0.0249	-0.0267
	H_8	0.0578	0.1659	0.0396	0.0232
	H_{10}	0.0095	0.0104	0.0083	0.0078
	H_{12}	0.0096	0.0101	0.0090	0.0084
	H_{13}	0.0008	0.0008	0.0009	0.0006
	H_{14}	0.0182	0.0193	0.0186	0.0138
	H_{15}	0.0183	0.0149	0.0163	0.0163
	X_{16}	0.0579	0.9085	0.0189	0.2083

Spin densities on the atoms of the X-toluene adducts (X=H, O(^{3}P), F and Cl).

Position	Atom	H	O	F	Cl
Meta	C_2	0.5518	0.5449	0.5428	0.5205
	C_4	0.4373	0.4487	0.4272	0.4083
	C_5	-0.0702	-0.0646	0.0088	-0.0542
	C_6	0.3975	0.3954	0.3750	0.3585
	C_7	0.0115	0.0103	0.0104	0.0112
	H_9	0.0096	0.0105	0.0088	0.0086
	H_{11}	0.0573	0.1654	0.0385	0.0266
	H_{13}	-0.0011	-0.0009	-0.0010	-0.0009
	H_{14}	-0.0053	-0.0045	-0.0052	-0.0043
	H_{15}	-0.0053	-0.0052	-0.0052	-0.0050
	X_{16}	0.0575	0.9194	0.0197	0.1773
Para	C_1	0.5228	0.5044	0.5035	0.5607
	C_3	0.4121	0.4111	0.3856	0.4110
	C_4	-0.0689	-0.0633	0.0121	-0.0527
	C_7	-0.0403	-0.0335	-0.0356	-0.0461
	H_8	0.0094	0.0087	0.0079	0.0085
	H_{10}	0.0548	0.1599	0.0340	0.0348
	H_{13}	0.0085	0.0082	0.0074	0.0085
	H_{14}	0.0085	0.0077	0.0096	0.0096
	H_{15}	0.0334	0.0325	0.0329	0.0347
	X_{16}	0.0569	0.9246	0.0224	0.0433

Spin densities on the atoms of the X-toluene adducts (X=H, O(^{3}P), F and Cl)

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Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.542500
3	6	2.336943	0.000000	3.254606
4	6	0.649560	1.244250	2.069865
5	6	0.649875	-1.244143	2.070298
6	6	1.747057	-1.222460	2.845876
7	6	1.746577	1.222525	2.844982
8	1	0.211475	2.189058	1.771244
9	1	0.211784	-2.189022	1.771909
10	1	2.187450	-2.153832	3.178802
11	1	2.187265	2.153880	3.177566
12	1	3.213262	0.002369	3.885500
13	1	-0.501473	-0.888389	-0.384765
14	1	1.024377	0.008289	-0.368283
15	1	-0.515862	0.880151	-0.384674
16	1	-1.057177	-0.000447	1.849316

MP2/6-31G** geometrical parameters of the *ipso* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.553511
3	6	2.234125	0.000000	3.436474
4	6	0.634680	1.250653	2.103189
5	6	0.634933	-1.250632	2.103136
6	6	1.683831	-1.224591	2.978210
7	6	1.683448	1.224550	2.978325
8	1	0.228520	2.201100	1.764511
9	1	0.228967	-2.201120	1.764337
10	1	2.107479	-2.160553	3.334541
11	1	2.106896	2.160501	3.334928
12	1	3.064870	0.000898	4.134111
13	1	-0.515570	-0.885051	-0.387667
14	1	1.024145	-0.002769	-0.383968
15	1	-0.510693	0.887905	-0.387595
16	1	-1.069662	-0.000060	1.843960

B3LYP/6-31G** geometrical parameters of the *ipso* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.033462	-0.000400	-0.011610
2	6	0.020292	-0.000442	1.526766
3	6	2.324827	0.001084	3.296751
4	6	0.675086	1.243771	2.046757
5	6	0.676822	-1.243812	2.046604
6	6	1.757132	-1.218169	2.866706
7	6	1.755451	1.219559	2.866877
8	1	0.256558	2.187163	1.730636
9	1	0.259616	-2.187748	1.730360
10	1	2.193353	-2.146845	3.200466
11	1	2.190323	2.148834	3.200731
12	1	3.182332	0.001588	3.947704
13	1	-0.554978	-0.880672	-0.379283
14	1	0.969548	0.000483	-0.428017
15	1	-0.556472	0.879027	-0.379180
16	1	-1.025316	-0.001193	1.862473

BH&HLYP/6-31G** geometrical parameters of the *ipso* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.344500
3	6	1.210452	0.000000	-0.733402
4	1	-0.940081	0.000445	-0.536909
5	6	1.268132	-0.000591	2.140019
6	6	2.448145	-0.000595	-0.039168
7	1	-0.933093	-0.000023	1.892674
8	1	1.194654	-0.000478	-1.813087
9	6	2.516735	-0.001048	1.303360
10	1	1.287831	-0.866060	2.820134
11	1	3.366829	-0.000629	-0.614560
12	1	1.288616	0.865258	2.819789
13	6	3.812501	-0.000724	2.051027
14	1	3.886502	-0.875706	2.701688
15	1	3.889170	0.878236	2.695993
16	1	4.664343	-0.004149	1.373234

MP2/6-31G** geometrical parameters of the *ortho* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.365495
3	6	1.213681	0.000000	-0.733665
4	1	-0.944805	-0.000177	-0.537912
5	6	1.274304	0.000458	2.159859
6	6	2.452532	-0.000150	-0.044641
7	1	-0.936498	-0.000826	1.916881
8	1	1.196660	-0.000305	-1.818402
9	6	2.530425	0.000036	1.323325
10	1	1.291550	-0.865235	2.850956
11	1	3.374435	-0.000147	-0.622892
12	1	1.291577	0.867019	2.849917
13	6	3.836443	0.000282	2.061020
14	1	3.925866	-0.877505	2.716815
15	1	3.927063	0.880064	2.713995
16	1	4.689601	-0.001323	1.376853

B3LYP/6-31G** geometrical parameters of the *ortho* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.002022	-0.000046	-0.007303
2	6	0.000066	0.000153	1.349063
3	6	1.211074	-0.000545	-0.734748
4	1	-0.934531	0.000168	-0.542628
5	6	1.265950	-0.000128	2.143385
6	6	2.443399	-0.000836	-0.045721
7	1	-0.930907	0.000516	1.893411
8	1	1.196533	-0.000709	-1.811246
9	6	2.515545	-0.000651	1.311787
10	1	1.281599	-0.861917	2.823147
11	1	3.359041	-0.001240	-0.617925
12	1	1.282130	0.861864	2.822884
13	6	3.812780	-0.000696	2.050913
14	1	3.896803	-0.873320	2.699590
15	1	3.898249	0.873652	2.697102
16	1	4.660984	-0.002326	1.373582

BH&HLYP/6-31G** geometrical parameters of the *ortho* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.496115
3	6	1.143442	0.000000	-0.711032
4	1	-0.957881	-0.000076	-0.503268
5	6	1.376376	-0.000451	2.086983
6	6	2.405884	0.000025	-0.078300
7	1	-0.566094	0.865769	1.869166
8	1	1.101577	0.000309	-1.793052
9	1	-0.566054	-0.866112	1.868656
10	6	2.494926	-0.000382	1.348762
11	1	1.446625	-0.000820	3.168414
12	1	3.310905	-0.000705	-0.670022
13	6	3.861899	-0.000270	1.978599
14	1	3.795091	-0.001386	3.064902
15	1	4.428691	0.879168	1.671335
16	1	4.429578	-0.878544	1.669605

MP2/6-31G** geometrical parameters of the *meta* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.030714	-0.045179	0.006942
2	6	-0.019796	-0.042510	1.507269
3	6	1.128468	-0.010922	-0.716685
4	1	-0.993868	-0.075667	-0.495176
5	6	1.360757	0.002334	2.097322
6	6	2.395493	0.029446	-0.086218
7	1	-0.620878	0.805332	1.888761
8	1	1.082470	-0.014300	-1.803184
9	1	-0.565427	-0.926146	1.891217
10	6	2.497663	0.036038	1.338267
11	1	1.437507	0.007348	3.182326
12	1	3.299295	0.055762	-0.687771
13	6	3.867567	0.080403	1.974440
14	1	3.804468	0.083188	3.065902
15	1	4.418091	0.976879	1.665602
16	1	4.471619	-0.783698	1.673344

B3LYP/6-31G** geometrical parameters of the *meta* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.005695	-0.000021	0.003017
2	6	-0.003136	-0.000275	1.496392
3	6	1.148519	0.000045	-0.711915
4	1	-0.959573	0.000101	-0.499834
5	6	1.369872	-0.000384	2.088163
6	6	2.406846	-0.000103	-0.078494
7	1	-0.569154	0.861743	1.870231
8	1	1.106907	0.000208	-1.790074
9	1	-0.569159	-0.862419	1.869931
10	6	2.501706	-0.000301	1.340134
11	1	1.441490	-0.000545	3.165205
12	1	3.307284	-0.000049	-0.670822
13	6	3.862984	-0.000365	1.976018
14	1	3.795727	-0.001097	3.059119
15	1	4.434948	0.875136	1.675497
16	1	4.435419	-0.875151	1.674330

BH&HLYP/6-31G** geometrical parameters of the *meta* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.498002
3	1	1.016446	0.000000	-0.403863
4	1	-0.505013	0.881890	-0.393775
5	1	-0.505018	-0.881886	-0.393775
6	6	0.035565	-1.217042	2.232484
7	6	0.036048	1.217028	2.232466
8	6	0.093277	1.246223	3.573147
9	6	0.092777	-1.246243	3.573160
10	1	0.005792	-2.150090	1.680999
11	1	0.006628	2.150085	1.680975
12	6	0.136463	-0.000013	4.402639
13	1	0.110913	2.194327	4.094952
14	1	0.110052	-2.194335	4.094999
15	1	1.036587	-0.000200	5.034791
16	1	-0.693277	0.000179	5.124202

MP2/6-31G** geometrical parameters of the *para* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.006532	-0.000112	-0.015146
2	6	0.000582	0.000277	1.488485
3	1	1.029452	-0.000351	-0.420052
4	1	-0.494549	0.885552	-0.419944
5	1	-0.494784	-0.885852	-0.419484
6	6	0.017923	-1.218964	2.225512
7	6	0.018506	1.219888	2.224877
8	6	0.057534	1.252375	3.588449
9	6	0.056930	-1.250763	3.589096
10	1	-0.003712	-2.156804	1.673383
11	1	-0.002689	2.157455	1.672267
12	6	0.088446	0.001016	4.418608
13	1	0.064407	2.205473	4.110806
14	1	0.063335	-2.203580	4.111969
15	1	0.980131	0.000963	5.075155
16	1	-0.752049	0.001416	5.138791

B3LYP/6-31G** geometrical parameters of the *para* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.002316	-0.000003	-0.001231
2	6	0.010597	-0.000004	1.494595
3	1	1.008329	-0.000009	-0.412544
4	1	-0.506395	0.878874	-0.394418
5	1	-0.506412	-0.878869	-0.394417
6	6	0.037686	-1.214029	2.226579
7	6	0.038163	1.214020	2.226565
8	6	0.094493	1.245090	3.579981
9	6	0.094003	-1.245102	3.579997
10	1	0.009240	-2.144076	1.678344
11	1	0.010084	2.144073	1.678319
12	6	0.135449	-0.000009	4.406423
13	1	0.108761	2.190527	4.098711
14	1	0.107898	-2.190538	4.098740
15	1	1.030298	-0.000181	5.040686
16	1	-0.692635	0.000158	5.125075

BH&HLYP/6-31G** geometrical parameters of the *para* H-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.557589
3	6	2.399096	0.000000	3.155758
4	6	0.655694	1.248876	2.065845
5	6	0.655694	-1.248876	2.065846
6	6	1.784536	-1.224209	2.794572
7	6	1.784536	1.224209	2.794570
8	1	0.164539	2.178469	1.808523
9	1	0.164538	-2.178469	1.808525
10	1	2.229651	-2.153041	3.127345
11	1	2.229652	2.153041	3.127342
12	1	3.304582	0.000000	3.744119
13	1	-0.508062	-0.889590	-0.368127
14	1	1.033472	0.000000	-0.337117
15	1	-0.508062	0.889590	-0.368126
16	8	-1.373397	0.000002	1.846152

MP2/6-31G** geometrical parameters of the *ipso* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.003876	-0.000951	-0.018940
2	6	-0.040020	0.000176	1.565918
3	6	2.301690	0.002943	3.294434
4	6	0.611850	1.259043	2.085869
5	6	0.613431	-1.257073	2.087820
6	6	1.717290	-1.224760	2.892379
7	6	1.715813	1.229314	2.890403
8	1	0.139781	2.194586	1.799933
9	1	0.142577	-2.193689	1.803422
10	1	2.147845	-2.157540	3.247854
11	1	2.145304	2.163152	3.244361
12	1	3.175364	0.003967	3.937691
13	1	-0.494808	-0.894151	-0.401790
14	1	1.052387	-0.000473	-0.324986
15	1	-0.496110	0.890894	-0.403244
16	8	-1.410145	-0.000534	1.794830

B3LYP/6-31G** geometrical parameters of the *ipso* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.010996	-0.000002	-0.004798
2	6	-0.002642	0.000001	1.553407
3	6	2.395077	0.000001	3.174798
4	6	0.658543	1.248752	2.058327
5	6	0.658543	-1.248754	2.058327
6	6	1.791905	-1.220816	2.803305
7	6	1.791904	1.220818	2.803305
8	1	0.178593	2.178108	1.797202
9	1	0.178592	-2.178111	1.797202
10	1	2.234163	-2.147156	3.134032
11	1	2.234165	2.147159	3.134032
12	1	3.293107	0.000001	3.768432
13	1	-0.519850	-0.884641	-0.372861
14	1	1.014676	-0.000007	-0.355710
15	1	-0.519842	0.884647	-0.372858
16	8	-1.359455	0.000000	1.846683

BH&HLYP/6-31G** geometrical parameters of the O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.344627
3	6	1.211145	0.000000	-0.729790
4	1	-0.939268	-0.002562	-0.537657
5	6	1.271409	0.028538	2.133695
6	6	2.449129	0.036289	-0.043388
7	1	-0.918148	0.019597	1.915350
8	1	1.193541	0.001450	-1.809582
9	6	2.526833	0.042262	1.300699
10	1	1.308749	-0.856774	2.809456
11	1	3.364092	0.055360	-0.623874
12	8	1.257722	1.061705	3.087029
13	6	3.815708	0.083570	2.056397
14	1	3.907114	-0.787225	2.710636
15	1	3.854498	0.965452	2.695072
16	1	4.668041	0.096449	1.380132

MP2/6-31G** geometrical parameters of the *ortho* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.365383
3	6	1.213327	0.000000	-0.732326
4	1	-0.945137	0.009883	-0.536806
5	6	1.281884	0.020927	2.156115
6	6	2.455277	0.020708	-0.052810
7	1	-0.920109	0.026830	1.940489
8	1	1.192556	0.003154	-1.817030
9	6	2.546513	0.024404	1.315282
10	1	1.312171	-0.897134	2.810254
11	1	3.372343	0.041720	-0.637875
12	8	1.274302	1.005457	3.138018
13	6	3.846538	0.048746	2.058662
14	1	3.967519	-0.852955	2.676354
15	1	3.882554	0.900424	2.746721
16	1	4.698709	0.108477	1.376849

B3LYP/6-31G** geometrical parameters of the *ortho* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.001795	0.000873	-0.006695
2	6	-0.000915	0.019962	1.349104
3	6	1.211897	-0.008725	-0.731091
4	1	-0.934154	0.002825	-0.542440
5	6	1.268358	0.032351	2.141044
6	6	2.444740	0.025734	-0.047965
7	1	-0.917377	0.052024	1.914558
8	1	1.196123	-0.021722	-1.807453
9	6	2.525109	0.048993	1.310217
10	1	1.296374	-0.874246	2.784465
11	1	3.357515	0.041334	-0.623899
12	8	1.256890	1.023434	3.111138
13	6	3.816490	0.093574	2.055606
14	1	3.928127	-0.780563	2.698371
15	1	3.855993	0.964044	2.705488
16	1	4.663625	0.124220	1.378391

BH&HLYP/6-31G** geometrical parameters of the *ortho* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.496604
3	6	1.149262	0.000000	-0.703851
4	1	-0.965519	-0.033408	-0.485173
5	6	1.370638	-0.016782	2.100426
6	6	2.404018	0.016085	-0.060504
7	1	-0.547753	0.898194	1.859690
8	1	1.116170	-0.012670	-1.785716
9	8	-0.817366	-1.016270	2.020230
10	6	2.491927	-0.016633	1.365136
11	1	1.410730	-0.060954	3.181514
12	1	3.311938	0.013257	-0.648002
13	6	3.856751	-0.055845	1.998148
14	1	3.785615	-0.069169	3.083685
15	1	4.443145	0.814784	1.703433
16	1	4.403927	-0.943177	1.679200

MP2/6-31G** geometrical parameters of the *meta* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.019715	-0.038945	-0.010819
2	6	-0.006757	-0.029638	1.494630
3	6	1.142950	0.004298	-0.728657
4	1	-0.989955	-0.114612	-0.491211
5	6	1.375145	0.019624	2.092392
6	6	2.404415	0.068279	-0.091248
7	1	-0.575245	0.877656	1.845705
8	1	1.103160	-0.022585	-1.814732
9	8	-0.801585	-1.029184	2.046588
10	6	2.511172	0.059982	1.332285
11	1	1.426594	-0.011789	3.177141
12	1	3.308825	0.098447	-0.691801
13	6	3.882308	0.079300	1.967256
14	1	3.818999	0.075462	3.058238
15	1	4.444297	0.970249	1.664019
16	1	4.471918	-0.791935	1.659559

B3LYP/6-31G** geometrical parameters of the *meta* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.006254	-0.014746	0.003065
2	6	-0.005614	-0.006805	1.498525
3	6	1.152590	0.001450	-0.704205
4	1	-0.967299	-0.051511	-0.482343
5	6	1.364295	-0.031928	2.100975
6	6	2.405114	0.016802	-0.061044
7	1	-0.527140	0.910822	1.846165
8	1	1.118797	-0.009460	-1.782216
9	8	-0.835118	-0.981387	2.032104
10	6	2.498594	-0.017733	1.356460
11	1	1.406745	-0.080783	3.177360
12	1	3.307821	0.026704	-0.649834
13	6	3.857332	-0.053995	1.996550
14	1	3.784913	-0.075958	3.078726
15	1	4.443959	0.818199	1.716019
16	1	4.414756	-0.932258	1.678472

BH&HLYP/6-31G** geometrical parameters of the *meta* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000233	0.000074	0.000055
2	6	0.000361	0.001082	1.498028
3	1	1.015879	0.010738	-0.393251
4	1	-0.525510	0.869793	-0.393199
5	1	-0.497033	-0.888835	-0.396612
6	6	1.070823	-0.576106	2.229487
7	6	-1.118435	0.492471	2.224220
8	6	-1.169472	0.468985	3.565106
9	6	1.077566	-0.626723	3.572309
10	1	1.912498	-0.978010	1.677491
11	1	-1.950585	0.906498	1.666643
12	6	-0.064123	-0.110776	4.391770
13	1	-2.033001	0.835104	4.103512
14	1	1.895430	-1.079818	4.115606
15	1	0.308751	0.659191	5.102582
16	8	-0.537391	-1.075127	5.299813

MP2/6-31G** geometrical parameters of the *para* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.012843	-0.001566	-0.005545
2	6	0.001296	-0.000212	1.497553
3	1	1.039478	-0.001958	-0.399057
4	1	-0.480847	0.887499	-0.412792
5	1	-0.488766	-0.884900	-0.411529
6	6	-0.187486	-1.202528	2.234527
7	6	0.191727	1.210736	2.225348
8	6	0.229937	1.247548	3.588051
9	6	-0.160606	-1.237443	3.599377
10	1	-0.371658	-2.123191	1.684678
11	1	0.297458	2.138990	1.667237
12	6	0.055017	0.005592	4.422048
13	1	0.347157	2.182268	4.127637
14	1	-0.334878	-2.158160	4.147470
15	1	0.977379	-0.136810	5.052808
16	8	-0.892276	0.158733	5.429932

B3LYP/6-31G** geometrical parameters of the *para* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.011547	-0.024353	0.005549
2	6	-0.010875	-0.019955	1.500909
3	1	0.999222	-0.013752	-0.392115
4	1	-0.540799	0.836615	-0.393927
5	1	-0.503940	-0.914436	-0.387831
6	6	1.070975	-0.562587	2.235363
7	6	-1.108346	0.501399	2.229747
8	6	-1.159861	0.481778	3.581277
9	6	1.080974	-0.612257	3.587804
10	1	1.924575	-0.938731	1.691710
11	1	-1.927178	0.942199	1.681097
12	6	-0.061377	-0.105244	4.423267
13	1	-2.005609	0.891906	4.107625
14	1	1.922068	-1.025813	4.118863
15	1	0.306874	0.653238	5.124141
16	8	-0.589165	-1.181466	5.150083

BH&HLYP/6-31G** geometrical parameters of the *para* O-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.001532	-0.000179	0.000358
2	6	-0.000832	-0.000449	1.525403
3	6	2.298358	0.001030	3.258898
4	6	0.616864	1.244876	2.074337
5	6	0.618729	-1.244937	2.074034
6	6	1.705102	-1.223695	2.862501
7	6	1.703188	1.225065	2.862732
8	1	0.146119	2.175310	1.784654
9	1	0.149340	-2.175986	1.784114
10	1	2.133124	-2.152668	3.215952
11	1	2.129920	2.154521	3.216483
12	1	3.171611	0.001504	3.894051
13	1	-0.515408	-0.886412	-0.365846
14	1	1.023046	0.000090	-0.374973
15	1	-0.515763	0.885988	-0.365530
16	9	-1.379161	-0.001560	1.899318

MP2/6-31G** geometrical parameters of the *ipso* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.534155
3	6	2.222323	0.000000	3.408071
4	6	0.613338	1.250045	2.094200
5	6	0.614030	-1.250000	2.093925
6	6	1.665722	-1.226512	2.964717
7	6	1.664966	1.226417	2.964939
8	1	0.174420	2.188479	1.766986
9	1	0.175352	-2.188455	1.766445
10	1	2.078746	-2.160988	3.335089
11	1	2.077720	2.160880	3.335664
12	1	3.053628	0.001314	4.105245
13	1	-0.520541	-0.888175	-0.370733
14	1	1.020907	-0.000019	-0.391542
15	1	-0.520503	0.888183	-0.370783
16	9	-1.385840	-0.000482	1.900117

B3LYP/6-31G** geometrical parameters of the *ipso* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.012250	-0.000202	-0.002210
2	6	-0.002362	-0.000388	1.520645
3	6	2.293525	0.000999	3.277996
4	6	0.621357	1.243596	2.065811
5	6	0.623103	-1.243635	2.065495
6	6	1.712733	-1.219871	2.871662
7	6	1.711018	1.221157	2.871971
8	1	0.162381	2.173793	1.771510
9	1	0.165432	-2.174400	1.770959
10	1	2.138143	-2.146924	3.221407
11	1	2.135129	2.148716	3.221952
12	1	3.158392	0.001526	3.919088
13	1	-0.530918	-0.882092	-0.367057
14	1	0.999482	0.000560	-0.394581
15	1	-0.532158	0.881051	-0.366833
16	9	-1.357240	-0.001388	1.898669

BH&HLYP/6-31G** geometrical parameters of the *ipso* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.343200
3	6	1.214416	0.000000	-0.727404
4	1	-0.937719	0.004363	-0.540005
5	6	1.263213	-0.022965	2.131730
6	6	2.448804	0.052301	-0.034770
7	1	-0.921199	0.014918	1.909220
8	1	1.200388	0.000140	-1.807212
9	6	2.512766	0.057718	1.309105
10	1	1.301732	-0.918028	2.768784
11	1	3.366869	0.096596	-0.608501
12	9	1.255472	1.063350	3.052246
13	6	3.789655	0.149231	2.080474
14	1	3.895295	-0.703577	2.755258
15	1	3.789219	1.046062	2.699457
16	1	4.651955	0.175883	1.417546

MP2/6-31G** geometrical parameters of the *ortho* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.365093
3	6	1.217780	0.000000	-0.726398
4	1	-0.942496	0.007556	-0.540720
5	6	1.266576	-0.022880	2.155104
6	6	2.453611	0.029158	-0.037095
7	1	-0.925740	0.014413	1.932247
8	1	1.203937	0.001467	-1.811250
9	6	2.524000	0.034146	1.332322
10	1	1.293697	-0.916380	2.804298
11	1	3.376404	0.060262	-0.611885
12	9	1.264828	1.066571	3.076752
13	6	3.813751	0.099165	2.092560
14	1	3.929547	-0.771976	2.752426
15	1	3.830343	0.982105	2.741443
16	1	4.676846	0.138717	1.423177

B3LYP/6-31G** geometrical parameters of the *ortho* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.002214	0.000378	-0.006993
2	6	0.000050	0.012408	1.348203
3	6	1.214993	-0.002015	-0.728747
4	1	-0.932398	0.003022	-0.544608
5	6	1.260174	-0.016670	2.137752
6	6	2.444018	0.046413	-0.039570
7	1	-0.919347	0.032136	1.909837
8	1	1.202898	-0.011436	-1.805187
9	6	2.510324	0.063344	1.318960
10	1	1.292323	-0.920338	2.755225
11	1	3.360161	0.084286	-0.608617
12	9	1.250732	1.035075	3.062911
13	6	3.790132	0.154529	2.080045
14	1	3.912594	-0.700784	2.745005
15	1	3.795114	1.041334	2.709319
16	1	4.646884	0.194313	1.415595

BH&HLYP/6-31G** geometrical parameters of the *ortho* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.490174
3	6	1.145188	0.000000	-0.708861
4	1	-0.965300	-0.007389	-0.486626
5	6	1.362599	-0.076421	2.089773
6	6	2.400578	-0.013029	-0.066286
7	1	-0.529471	0.884926	1.866889
8	1	1.109960	0.007241	-1.790488
9	9	-0.772107	-1.100894	1.951159
10	6	2.485522	-0.076322	1.360473
11	1	1.403190	-0.137824	3.169985
12	1	3.308999	-0.014221	-0.652932
13	6	3.848370	-0.148247	1.993442
14	1	3.775351	-0.189718	3.078084
15	1	4.445783	0.722699	1.722682
16	1	4.384771	-1.033405	1.651116

MP2/6-31G** geometrical parameters of the *meta* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.019471	-0.024050	0.000795
2	6	-0.006120	0.030284	1.493408
3	6	1.138055	0.002382	-0.726113
4	1	-0.990489	-0.083924	-0.480923
5	6	1.365732	0.037746	2.086344
6	6	2.401033	0.057149	-0.091250
7	1	-0.568309	0.914864	1.840821
8	1	1.093941	-0.029593	-1.811548
9	9	-0.740205	-1.071800	2.013590
10	6	2.506228	0.060751	1.332674
11	1	1.418998	0.025181	3.171646
12	1	3.305770	0.072245	-0.692043
13	6	3.875429	0.076816	1.970166
14	1	3.809541	0.073770	3.061021
15	1	4.441681	0.965512	1.668050
16	1	4.462665	-0.796653	1.664315

B3LYP/6-31G** geometrical parameters of the *meta* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.006400	-0.013493	0.003506
2	6	-0.004678	-0.005530	1.491063
3	6	1.148677	0.000307	-0.708908
4	1	-0.967847	-0.022734	-0.482679
5	6	1.355543	-0.090694	2.089222
6	6	2.402000	-0.014216	-0.066850
7	1	-0.510989	0.893481	1.854865
8	1	1.112497	0.011121	-1.786605
9	9	-0.787202	-1.064177	1.962725
10	6	2.492644	-0.078672	1.350608
11	1	1.397658	-0.155908	3.164883
12	1	3.305078	-0.005083	-0.655015
13	6	3.849153	-0.146140	1.991822
14	1	3.773950	-0.198115	3.072740
15	1	4.445096	0.727777	1.737467
16	1	4.398253	-1.020528	1.649739

BH&HLYP/6-31G** geometrical parameters of the *meta* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.497316
3	1	1.015814	0.000000	-0.393331
4	1	-0.518607	0.873446	-0.393357
5	1	-0.504279	-0.885865	-0.394881
6	6	1.035209	-0.643623	2.227729
7	6	-1.081840	0.561456	2.227797
8	6	-1.125983	0.535896	3.568417
9	6	1.035894	-0.694659	3.568309
10	1	1.849826	-1.096050	1.674473
11	1	-1.886836	1.030947	1.674662
12	6	-0.054668	-0.096327	4.388769
13	1	-1.960586	0.962239	4.107936
14	1	1.828614	-1.194645	4.107771
15	1	0.356333	0.625663	5.105168
16	9	-0.633143	-1.112695	5.200063

MP2/6-31G** geometrical parameters of the *para* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.502663
3	1	1.017750	0.000000	-0.402220
4	1	-0.526898	0.871404	-0.402082
5	1	-0.504465	-0.891114	-0.400360
6	6	1.073606	-0.579126	2.236850
7	6	-1.102095	0.528585	2.234397
8	6	-1.144903	0.507101	3.597697
9	6	1.078696	-0.624819	3.600749
10	1	1.911073	-1.001040	1.685493
11	1	-1.934517	0.957555	1.680772
12	6	-0.037484	-0.065355	4.420583
13	1	-1.998800	0.906224	4.136879
14	1	1.902467	-1.080375	4.142053
15	1	0.347780	0.693592	5.122430
16	9	-0.558271	-1.085949	5.268316

B3LYP/6-31G** geometrical parameters of the *para* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.006327	0.011041	-0.001888
2	6	-0.005474	-0.009510	1.493516
3	1	1.020733	0.014849	-0.390700
4	1	-0.508330	0.885111	-0.390960
5	1	-0.493237	-0.866681	-0.413778
6	6	1.028183	-0.649227	2.221892
7	6	-1.083233	0.552527	2.222027
8	6	-1.135179	0.515878	3.575036
9	6	1.023373	-0.712688	3.574886
10	1	1.839198	-1.104162	1.673729
11	1	-1.888447	1.017778	1.673989
12	6	-0.054863	-0.096663	4.394334
13	1	-1.969609	0.937408	4.111108
14	1	1.811725	-1.215220	4.110888
15	1	0.370172	0.649934	5.070678
16	9	-0.605592	-1.064592	5.242084

BH&HLYP/6-31G** geometrical parameters of the *para* F-toluene adduct.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.037232	-0.000213	-0.024338
2	6	0.062041	-0.000342	1.498870
3	6	2.267298	0.000971	3.349665
4	6	0.702810	1.240535	2.012057
5	6	0.704560	-1.240448	2.011732
6	6	1.729854	-1.219973	2.880358
7	6	1.728131	1.221279	2.880678
8	1	0.293260	2.175469	1.652465
9	1	0.296331	-2.175865	1.651894
10	1	2.157439	-2.152163	3.225409
11	1	2.154400	2.153981	3.225973
12	1	3.087032	0.001458	4.052471
13	1	-0.567364	-0.885943	-0.370830
14	1	0.968552	0.000552	-0.444077
15	1	-0.568613	0.884860	-0.370598
16	17	-1.692728	-0.001661	2.114758

MP2/6-31G** geometrical parameters of the *ipso* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.084090	-0.000241	-0.044636
2	6	0.127678	-0.000292	1.459726
3	6	2.240213	0.000944	3.404539
4	6	0.754495	1.237226	1.967630
5	6	0.756248	-1.237057	1.967299
6	6	1.739515	-1.215889	2.906197
7	6	1.737794	1.217199	2.906521
8	1	0.375128	2.168908	1.581807
9	1	0.378203	-2.169172	1.581224
10	1	2.150591	-2.145206	3.265556
11	1	2.147555	2.147002	3.266126
12	1	3.015880	0.001393	4.151092
13	1	-0.634758	-0.881300	-0.355528
14	1	0.884041	0.000477	-0.539703
15	1	-0.635952	0.880152	-0.355297
16	17	-1.666771	-0.001663	2.183917

BHandHLYP/6-31G** geometrical parameters of the *ipso* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.344794
3	6	1.213687	0.000000	-0.720920
4	1	-0.937511	-0.026972	-0.539162
5	6	1.256657	0.093603	2.121522
6	6	2.441401	-0.050921	-0.026321
7	1	-0.924217	-0.010281	1.905558
8	1	1.204272	0.004993	-1.800931
9	6	2.503515	-0.049932	1.320798
10	1	1.258921	-0.586228	2.975055
11	1	3.359995	-0.124472	-0.595738
12	17	1.276017	1.749097	2.986783
13	6	3.790289	-0.157757	2.075005
14	1	3.763067	-1.006040	2.762533
15	1	3.963094	0.736503	2.674704
16	1	4.630703	-0.291670	1.396988

MP2/6-31G** geometrical parameters of the *ortho* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.034039	-0.022288	0.004197
2	6	0.039836	-0.038650	1.364248
3	6	1.242847	-0.002858	-0.713123
4	1	-0.902221	-0.043838	-0.528851
5	6	1.292133	0.051821	2.117892
6	6	2.468208	-0.046461	-0.030286
7	1	-0.878157	-0.062503	1.926063
8	1	1.230497	0.013778	-1.789708
9	6	2.534645	-0.064354	1.335015
10	1	1.299986	-0.547489	3.018743
11	1	3.383776	-0.091570	-0.598535
12	17	1.295154	1.811991	2.975216
13	6	3.825925	-0.158780	2.077811
14	1	3.825365	-1.011654	2.755494
15	1	3.986621	0.729352	2.684947
16	1	4.664056	-0.267703	1.397872

BHandHLYP/6-31G** geometrical parameters of the *ortho* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.481424
3	6	1.151235	0.000000	-0.702294
4	1	-0.959149	-0.045428	-0.496098
5	6	1.341432	0.170718	2.088357
6	6	2.398382	0.067390	-0.054424
7	1	-0.714921	0.719738	1.881847
8	1	1.120269	-0.033697	-1.783412
9	17	-0.729720	-1.603059	2.074934
10	6	2.471671	0.173260	1.366345
11	1	1.377734	0.255407	3.166868
12	1	3.311124	0.059500	-0.634428
13	6	3.824340	0.305799	2.010627
14	1	3.736698	0.400564	3.090791
15	1	4.350746	1.180957	1.629405
16	1	4.438392	-0.568317	1.792805

MP2/6-31G** geometrical parameters of the *meta* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.001146	0.040199	-0.003227
2	6	0.012071	0.053903	1.465483
3	6	1.164849	0.017228	-0.709663
4	1	-0.954272	0.003337	-0.497690
5	6	1.337333	0.216359	2.079442
6	6	2.407233	0.072878	-0.059029
7	1	-0.733857	0.713919	1.889411
8	1	1.134569	-0.029963	-1.786090
9	17	-0.714857	-1.625211	2.066955
10	6	2.486152	0.192023	1.350714
11	1	1.372034	0.312551	3.152013
12	1	3.315723	0.048178	-0.638539
13	6	3.832598	0.303143	2.005774
14	1	3.741104	0.440625	3.077811
15	1	4.396572	1.141699	1.604016
16	1	4.421380	-0.594960	1.832775

BHandHLYP/6-31G** geometrical parameters of the *meta* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.000000	0.000000	0.000000
2	6	0.000000	0.000000	1.497200
3	1	1.015636	0.000000	-0.393499
4	1	-0.520404	0.872493	-0.393355
5	1	-0.504038	-0.886554	-0.392657
6	6	1.059586	-0.592425	2.228090
7	6	-1.075306	0.567007	2.226453
8	6	-1.126719	0.525053	3.568213
9	6	1.050460	-0.657133	3.570300
10	1	1.912710	-0.976896	1.681892
11	1	-1.861271	1.073106	1.678643
12	6	-0.106547	-0.190671	4.366949
13	1	-1.948183	0.976488	4.106897
14	1	1.875563	-1.100000	4.110532
15	1	0.204908	0.384569	5.238716
16	17	-0.908075	-1.665161	5.182205

MP2/6-31G** geometrical parameters of the *para* Cl-toluene adducts.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.004537	-0.008525	-0.009712
2	6	0.001452	0.003521	1.485837
3	1	1.004763	-0.006358	-0.410954
4	1	-0.533088	0.851157	-0.411608
5	1	-0.502043	-0.900447	-0.390779
6	6	1.066109	-0.572622	2.212379
7	6	-1.061490	0.585229	2.210905
8	6	-1.100508	0.563911	3.569565
9	6	1.067876	-0.616026	3.571243
10	1	1.908715	-0.972406	1.670076
11	1	-1.853909	1.075574	1.667260
12	6	-0.075624	-0.133995	4.350657
13	1	-1.913192	1.022480	4.106543
14	1	1.893620	-1.049213	4.109365
15	1	0.204332	0.381706	5.259076
16	17	-0.919970	-1.684056	5.170585

BHandHLYP/6-31G** geometrical parameters of the *para* Cl-toluene adducts.

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.057534	-0.03072	-12.32291
2	C	0.421761	0.03626	14.54474
3	C	-0.189922	-0.03588	-14.39426
4	C	0.542035	0.04641	18.61717
5	C	-0.189906	-0.03589	-14.39612
6	C	0.421858	0.03627	14.54938
7	C	0.056764	0.07984	32.02784
8	H	-0.023143	-0.00667	-10.64437
9	H	0.009560	0.00272	4.33355
10	H	-0.030759	-0.00860	-13.70931
11	H	0.009561	0.00272	4.33450
12	H	-0.023152	-0.00668	-10.64710
13	H	0.000179	-0.00022	-0.35170
14	H	-0.001875	-0.00108	-1.72160
15	H	0.000177	-0.00022	-0.35153
16	H	0.054395	0.03200	51.03408

Hydrogen, ipso, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.062374	-0.04631	-9.28817
2	C	0.406667	0.03911	7.84489
3	C	-0.171960	-0.03122	-6.26110
4	C	0.555515	0.04531	9.08696
5	C	-0.171319	-0.03127	-6.27174
6	C	0.405975	0.03904	7.83043
7	C	0.107734	0.10733	21.52664
8	H	-0.020686	-0.00634	-5.05829
9	H	0.009138	0.00281	2.23758
10	H	-0.030525	-0.00857	-6.83491
11	H	0.009131	0.00281	2.23899
12	H	-0.020676	-0.00634	-5.05406
13	H	0.000077	0.00005	0.03814
14	H	0.014812	0.00805	6.42177
15	H	0.000075	0.00005	0.03613
16	O	0.968417	0.11326	-12.25030

Oxygen, ipso, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.005025	-0.01497	-6.00398
2	C	0.403796	0.03110	12.47436
3	C	-0.170422	-0.03115	-12.49442
4	C	0.525422	0.04049	16.24289
5	C	-0.170490	-0.03116	-12.49986
6	C	0.404216	0.03114	12.49081
7	C	0.032048	0.04251	17.05328
8	H	-0.020521	-0.00596	-9.50614
9	H	0.007765	0.00228	3.64099
10	H	-0.027754	-0.00778	-12.40607
11	H	0.007768	0.00228	3.64338
12	H	-0.020543	-0.00597	-9.51472
13	H	0.003870	0.00163	2.59206
14	H	-0.000161	0.00154	2.44943
15	H	0.003872	0.00163	2.59317
16	F	0.026159	0.07290	109.43903

Fluorine, ipso, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.049696	0.00182	0.7303
2	C	0.3947	0.02421	9.7099
3	C	-0.193093	-0.02747	-11.01787
4	C	0.5108	0.03187	12.7825
5	C	-0.193093	-0.02747	-11.01785
6	C	0.394697	0.02421	9.70984
7	C	0.013543	0.0309	12.39619
8	H	-0.020858	-0.00539	-8.60109
9	H	0.008364	0.00197	3.14514
10	H	-0.028541	-0.00693	-11.05143
11	H	0.008364	0.00197	3.14514
12	H	-0.020858	-0.00539	-8.60104
13	H	0.003131	0.00077	1.22699
14	H	0.001263	0.00048	0.77276
15	H	0.003131	0.00077	1.22673
16	Cl	0.168144	0.12797	20.02172

Chlorine, ipso, B3LYP/6-311G**

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.395807	0.03010	12.07232
2	C	-0.069425	-0.03011	-12.07639
3	C	0.423847	0.02915	11.69136
4	C	-0.189975	-0.03248	-13.02957
5	C	0.537999	0.03743	15.01481
6	C	-0.187845	-0.03255	-13.05806
7	C	-0.029199	-0.01382	-5.54218
8	H	0.057804	0.02897	46.20963
9	H	-0.022972	-0.00615	-9.80850
10	H	0.009537	0.00229	3.65978
11	H	-0.030290	-0.00781	-12.45403
12	H	0.009544	0.00224	3.57576
13	H	0.000791	0.00028	0.45298
14	H	0.018215	0.00792	12.63719
15	H	0.018263	0.00795	12.68154
16	H	0.057897	0.02902	46.28256

Hydrogen, ortho, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.408840	0.04525	9.07495
2	C	-0.050843	-0.05793	-11.61927
3	C	0.425801	0.04821	9.67009
4	C	-0.178696	-0.03115	-6.24673
5	C	0.524371	0.04386	8.79770
6	C	-0.181572	-0.03166	-6.34927
7	C	-0.027674	-0.01325	-2.65771
8	H	0.165930	0.08394	66.94056
9	H	-0.021391	-0.00668	-5.32913
10	H	0.010393	0.00333	2.65367
11	H	-0.028829	-0.00819	-6.53393
12	H	0.010113	0.00308	2.45571
13	H	0.000847	0.00042	0.33246
14	H	0.019329	0.00964	7.68503
15	H	0.014888	0.00971	7.74362
16	O	0.908491	0.11818	-12.78255

Oxygen, ortho, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.381268	0.03486	13.98424
2	C	0.021344	-0.01830	-7.34021
3	C	0.388190	0.03139	12.59247
4	C	-0.167258	-0.03182	-12.76389
5	C	0.513515	0.04080	16.36613
6	C	-0.177223	-0.03314	-13.29414
7	C	-0.024885	-0.01304	-5.23062
8	H	0.039563	0.02340	37.31626
9	H	-0.019671	-0.00578	-9.22130
10	H	0.008342	0.00254	4.05199
11	H	-0.026882	-0.00765	-12.20311
12	H	0.008973	0.00270	4.31400
13	H	0.000944	0.00051	0.81895
14	H	0.018597	0.00954	15.21697
15	H	0.016294	0.01036	16.52916
16	F	0.018891	0.07729	116.02968

Fluorine, ortho, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.364041	0.02375	9.5267
2	C	-0.043963	0.00965	3.86953
3	C	0.365322	0.02181	8.7493
4	C	-0.178979	-0.0254	-10.18905
5	C	0.475083	0.02953	11.84738
6	C	-0.187515	-0.02628	-10.54232
7	C	-0.026732	-0.01093	-4.38267
8	H	0.023201	0.01307	20.83982
9	H	-0.018943	-0.00501	-7.98382
10	H	0.007785	0.00183	2.92594
11	H	-0.026711	-0.00644	-10.26796
12	H	0.008435	0.002000	3.18942
13	H	0.000648	0.00025	0.39308
14	H	0.013775	0.00704	11.2231
15	H	0.01627	0.00835	13.31497
16	Cl	0.208282	0.14163	22.15867

Chlorine, ortho, B3LYP/6-311G**

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.170669	-0.03626	-14.54556
2	C	0.551769	0.04726	18.95636
3	C	-0.192818	-0.03689	-14.79804
4	C	0.437319	0.03732	14.96881
5	C	-0.070207	-0.03321	-13.32011
6	C	0.397548	0.03450	13.83918
7	C	0.011536	0.00540	2.16463
8	H	-0.031427	-0.00868	-13.83944
9	H	0.009645	0.00277	4.41698
10	H	-0.023723	-0.00697	-11.11726
11	H	0.057272	0.03383	53.95912
12	H	-0.021915	-0.00640	-10.21390
13	H	-0.001152	-0.00047	-0.75697
14	H	-0.005312	-0.00339	-5.40400
15	H	-0.005344	-0.00340	-5.42739
16	H	0.057479	0.03394	54.13366

Hydrogen, meta, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.159837	-0.03142	-6.30244
2	C	0.544899	0.04517	9.05983
3	C	-0.186873	-0.03237	-6.49177
4	C	0.448736	0.04854	9.73469
5	C	-0.064652	-0.05718	-11.46851
6	C	0.395374	0.04322	8.66939
7	C	0.010352	0.00523	1.04987
8	H	-0.030064	-0.0084	-6.70069
9	H	0.010519	0.00332	2.64952
10	H	-0.022507	-0.00697	-5.56211
11	H	0.165378	0.08492	67.72299
12	H	-0.020064	-0.0062	-4.94179
13	H	-0.000888	-0.00036	-0.28501
14	H	-0.004551	-0.0029	-2.31621
15	H	-0.005249	-0.00316	-2.51915
16	O	0.919426	0.1216	-13.15245

Oxygen, meta, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.162293	-0.03250	-13.03778
2	C	0.542811	0.04435	17.79190
3	C	-0.186054	-0.03368	-13.51088
4	C	0.427221	0.03511	14.08475
5	C	0.008853	-0.01709	-6.85381
6	C	0.375012	0.03158	12.66803
7	C	0.010426	0.00473	1.89644
8	H	-0.029705	-0.00832	-13.26587
9	H	0.008795	0.00256	4.08743
10	H	-0.022027	-0.00649	-10.35447
11	H	0.038509	0.02448	39.04399
12	H	-0.019772	-0.00575	-9.16645
13	H	-0.001009	-0.00041	-0.66175
14	H	-0.005208	-0.00316	-5.03351
15	H	-0.005254	-0.00308	-4.91099
16	F	0.019694	0.07998	120.07218

Fluorine, meta, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	-0.181365	-0.02647	-10.61734
2	C	0.520462	0.03199	12.83273
3	C	-0.196969	-0.0278	-11.14959
4	C	0.408338	0.02448	9.82078
5	C	-0.0542	0.00378	1.51477
6	C	0.358535	0.0212	8.5049
7	C	0.011207	0.0037	1.48532
8	H	-0.028555	-0.00695	-11.08582
9	H	0.008557	0.00202	3.21704
10	H	-0.02122	-0.00556	-8.86475
11	H	0.026594	0.01596	25.44959
12	H	-0.018428	-0.0048	-7.65711
13	H	-0.000924	-0.00034	-0.54152
14	H	-0.004308	-0.00243	-3.86921
15	H	-0.005049	-0.00269	-4.29799
16	Cl	0.177324	0.14234	22.26907

Chlorine, meta, B3LYP/6-311G**

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.522833	0.05008	20.08704
2	C	-0.187130	-0.03642	-14.60804
3	C	0.412073	0.03541	14.20224
4	C	-0.068929	-0.03278	-13.14764
5	C	0.412079	0.03541	14.20251
6	C	-0.187132	-0.03642	-14.60814
7	C	-0.040307	-0.01964	-7.87695
8	H	0.009451	0.00265	4.22704
9	H	-0.022320	-0.00660	-10.52880
10	H	0.054833	0.03269	52.14310
11	H	-0.022320	-0.00660	-10.52896
12	H	0.009451	0.00265	4.22711
13	H	0.008542	0.00494	7.87402
14	H	0.008536	0.00493	7.86885
15	H	0.033393	0.01878	29.94761
16	H	0.056946	0.03375	53.83272

Hydrogen, para, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.504419	0.04505	9.03462
2	C	-0.169674	-0.02919	-5.85450
3	C	0.411151	0.04412	8.84960
4	C	-0.063271	-0.05480	-10.99032
5	C	0.410149	0.04445	8.91506
6	C	-0.169054	-0.02912	-5.84074
7	C	-0.033475	-0.01702	-3.41319
8	H	0.008751	0.00262	2.08569
9	H	-0.020415	-0.00636	-5.07050
10	H	0.159915	0.08210	65.47141
11	H	-0.020329	-0.00635	-5.06074
12	H	0.008799	0.00263	2.10026
13	H	0.008191	0.00483	3.84996
14	H	0.007735	0.00454	3.62038
15	H	0.032517	0.01847	14.73264
16	O	0.924592	0.12437	-13.45154

Oxygen, para, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.503499	0.04505	18.07196
2	C	-0.168824	-0.03139	-12.59089
3	C	0.385636	0.03144	12.61278
4	C	0.012077	-0.01412	-5.66280
5	C	0.391013	0.03179	12.75017
6	C	-0.170098	-0.03160	-12.67397
7	C	-0.035583	-0.01782	-7.14806
8	H	0.007912	0.00224	3.57317
9	H	-0.019839	-0.00584	-9.31576
10	H	0.033982	0.02212	35.28231
11	H	-0.020071	-0.00591	-9.42767
12	H	0.007953	0.00225	3.59063
13	H	0.007377	0.00427	6.81496
14	H	0.009630	0.00563	8.97289
15	H	0.032933	0.01882	30.02444
16	F	0.022404	0.08647	129.81435

Fluorine, para, B3LYP/EPR-II

Center Number	Atom	spin densities	Fermi Contact (a.u.)	hcc (Gauss)
1	C	0.560655	0.03872	15.5339
2	C	-0.194904	-0.03005	-12.05374
3	C	0.410974	0.02556	10.25148
4	C	-0.052716	-0.02036	-8.16813
5	C	0.414268	0.02575	10.33098
6	C	-0.195864	-0.03018	-12.10436
7	C	-0.046111	-0.01785	-7.16006
8	H	0.00848	0.00194	3.09889
9	H	-0.022009	-0.00558	-8.90673
10	H	0.034798	0.01829	29.17001
11	H	-0.022188	-0.00563	-8.97629
12	H	0.008519	0.00195	3.11217
13	H	0.008507	0.0043	6.8516
14	H	0.009576	0.00486	7.74925
15	H	0.034693	0.01758	28.03831
16	Cl	0.043322	0.14745	23.06918

Chlorine, para, B3LYP/6-311G**