Detemination of The Best Method (HF, MP2 and B3LYP) in in Calculation of Chemical Hardness

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Supp. Table S1. Calculated chemical hardness values of mentioned molecules at HF/LANL2MB level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	7.172	BBr_3	6.834	C_5H_5N	7.366	cyclohexene	12.781
BF_3	11.181	PBr_3	4.979	butadiene	7.241	DMF	9.514
SO_3	4.447	S_2	3.760	H_2S	9.646	$C_6H_5NH_2$	6.972
Cl_2	5.912	$C_6H_5NO_2$	5.932	C_2H_2	10.522	$CH_3CH=C(CH_3)_2$	8.396
H_2	17.564	PCl_3	5.729	$HCONH_2$	8.586	CH_3F	13.804
SO_2	4.456	N_2O	7.927	styrene	6.555	H_2O	13.260
N_2	10.824	acrylonitrile	7.812	CH_3COCH_3	8.416	$(CH_3)_3As$	8.092
Br_2	5.059	CS_2	5.979	PH_3	9.666	$(CH_3)_3P$	8.628
O_2	7.041	CO_2	9.500	C_6H_6	7.529	$(CH_3)_2S$	8.615
CO	10.222	HF	14.327	toluene	7.372	NH_3	13.383
BCl_3	7.560	HCl	10.603	propylene	8.805	CH_4	16.868
CS	7.323	CH_3CN	10.459	C_6H_5OH	7.034	$C(CH_3)_4$	13.707
HNO_3	6.716	CH_2O	8.659	C_6H_5SH	7.178	$(CH_3)_2O$	12.203
CH_3NO_2	6.452	HCO_2CH_3	8.799	CH_3Cl	9.349	$(CH_3)_3N$	11.819
PF_3	7.972	CH_3CHO	8.542	p-xylene	7.231	-	-
HCN	10.767	C_2H_4	9.031	1,2,5-trimethylbenzene	7.189	-	-

Supp. Table S2. Calculated chemical hardness values of mentioned molecules at HF/SDD level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	7.963	BBr_3	6.200	C_5H_5N	6.290	cyclohexene	8.840
BF_3	10.908	PBr_3	5.067	butadiene	5.872	DMF	7.384
SO_3	6.329	S_2	3.830	H_2S	7.824	$C_6H_5NH_2$	5.693
Cl_2	5.903	$C_6H_5NO_2$	5.464	C_2H_2	8.043	$CH_3CH=C(CH_3)_2$	7.026
H_2	11.680	PCl_3	5.959	$HCONH_2$	7.955	CH_3F	10.317
SO_2	5.708	N_2O	8.282	styrene	5.425	H_2O	9.864
N_2	10.426	acrylonitrile	6.511	CH_3COCH_3	7.674	$(CH_3)_3As$	6.668
Br_2	6.405	CS_2	5.799	PH_3	7.642	$(CH_3)_3P$	7.189
O_2	6.735	CO_2	9.646	C_6H_6	6.341	$(CH_3)_2S$	7.235
CO	9.163	HF	11.633	toluene	6.168	NH_3	8.740
BCl_3	7.235	HCl	8.715	propylene	7.076	CH_4	11.497
CS	7.053	CH_3CN	9.053	C_6H_5OH	6.024	$C(CH_3)_4$	9.384
HNO_3	7.274	CH_2O	7.523	C_6H_5SH	6.238	$(CH_3)_2O$	8.847
CH_3NO_2	6.947	HCO_2CH_3	8.317	CH_3Cl	8.089	$(CH_3)_3N$	7.874
PF_3	8.231	CH_3CHO	7.628	p-xylene	6.031	-	-
HCN	9.084	C_2H_4	7.120	1,2,5-trimethylbenzene	6.056	-	-

Supp. Table S3. Calculated chemical hardness values of mentioned molecules at HF/SDDALL level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	7.680	BBr_3	6.226	C_5H_5N	6.434	cyclohexene	8.708
BF_3	11.161	PBr_3	5.041	butadiene	6.013	DMF	7.566
SO_3	6.042	S_2	3.750	H_2S	6.374	$C_6H_5NH_2$	5.818
Cl_2	5.927	$C_6H_5NO_2$	5.448	C_2H_2	8.332	$CH_3CH=C(CH_3)_2$	7.122
H_2	11.680	PCl_3	5.827	$HCONH_2$	8.077	CH_3F	10.510
SO_2	5.462	N_2O	8.421	styrene	5.572	H_2O	9.408
N_2	10.706	acrylonitrile	6.648	CH_3COCH_3	7.621	$(CH_3)_3As$	6.762
Br_2	5.063	CS_2	5.677	PH_3	7.468	$(CH_3)_3P$	6.999
O_2	6.674	CO_2	9.631	C_6H_6	6.495	$(CH_3)_2S$	5.736
CO	9.408	HF	11.597	toluene	6.328	NH_3	8.704
BCl_3	7.025	HCl	7.091	propylene	7.308	CH_4	11.821
CS	7.092	CH_3CN	9.147	C_6H_5OH	6.177	$C(CH_3)_4$	9.318
HNO_3	7.299	CH_2O	7.701	C_6H_5SH	5.885	$(CH_3)_2O$	8.629
CH_3NO_2	6.945	HCO_2CH_3	8.455	CH_3Cl	6.512	$(CH_3)_3N$	7.922
PF_3	8.065	CH_3CHO	7.706	p-xylene	6.182	-	-
HCN	9.417	C_2H_4	7.398	1,2,5-trimethylbenzene	6.198	-	-

Supp. Table S4. Calculated chemical hardness values of mentioned molecules at B3LYP/6-311G level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	2.488	BBr_3	2.825	C_5H_5N	2.959	cyclohexene	4.628
BF_3	5.785	PBr_3	2.092	butadiene	2.799	DMF	3.534
SO_3	2.256	S_2	0.440	H_2S	3.617	$C_6H_5NH_2$	2.725
Cl_2	1.839	$C_6H_5NO_2$	2.412	C_2H_2	4.560	$CH_3CH=C(CH_3)_2$	3.555
H_2	6.747	PCl_3	2.512	$HCONH_2$	3.669	CH_3F	5.308
SO_2	1.952	N_2O	4.019	styrene	2.602	H_2O	4.298
N_2	5.233	acrylonitrile	3.179	CH_3COCH_3	3.056	$(CH_3)_3As$	3.617
Br_2	1.607	CS_2	2.744	PH_3	4.011	$(CH_3)_3P$	3.619
O_2	0.947	CO_2	5.057	C_6H_6	3.401	$(CH_3)_2S$	3.390
CO	4.563	HF	5.524	toluene	3.263	NH_3	3.718
BCl_3	3.350	HCl	4.251	propylene	3.748	CH_4	6.128
CS	3.013	CH_3CN	4.960	C_6H_5OH	3.001	$C(CH_3)_4$	4.838
HNO_3	3.101	CH_2O	2.910	C_6H_5SH	3.104	$(CH_3)_2O$	4.049
CH_3NO_2	2.773	HCO_2CH_3	3.713	CH_3Cl	3.958	$(CH_3)_3N$	3.278
PF_3	4.067	CH_3CHO	3.034	p-xylene	3.141	-	-
HCN	5.166	C_2H_4	3.841	1,2,5-trimethylbenzene	3.149	-	-

Supp. Table S5. Calculated chemical hardness values of mentioned molecules at B3LYP/LANL2DZ level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	2.602	BBr_3	2.806	C_5H_5N	2.907	cyclohexene	5.778
BF_3	5.610	PBr_3	1.987	butadiene	2.713	DMF	3.472
SO_3	2.211	S_2	0.436	H_2S	3.949	$C_6H_5NH_2$	2.670
Cl_2	1.802	$C_6H_5NO_2$	2.343	C_2H_2	4.364	$CH_3CH=C(CH_3)_2$	3.541
H_2	7.409	PCl_3	3.397	$HCONH_2$	3.572	CH_3F	5.483
SO_2	1.902	N_2O	3.891	styrene	2.533	H_2O	4.905
N_2	4.987	acrylonitrile	3.090	CH_3COCH_3	3.048	$(CH_3)_3As$	3.652
Br_2	1.507	CS_2	2.726	PH_3	4.205	$(CH_3)_3P$	3.865
O_2	0.931	CO_2	4.960	C_6H_6	3.568	$(CH_3)_2S$	3.499
CO	4.381	HF	6.005	toluene	3.189	NH_3	4.431
BCl_3	2.508	HCl	4.580	propylene	3.636	CH_4	7.345
CS	2.932	CH_3CN	4.913	C_6H_5OH	3.168	$C(CH_3)_4$	5.661
HNO_3	3.003	CH_2O	2.835	C_6H_5SH	2.826	$(CH_3)_2O$	4.500
CH_3NO_2	2.713	HCO_2CH_3	3.624	CH_3Cl	4.048	$(CH_3)_3N$	4.032
PF_3	4.116	CH_3CHO	2.976	p-xylene	3.070	-	-
HCN	4.990	C_2H_4	3.701	1,2,5-trimethylbenzene	3.089	-	-

Supp. Table S6. Calculated chemical hardness values of mentioned molecules at B3LYP/LANL2MB level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	2.190	BBr_3	2.973	C_5H_5N	3.186	cyclohexene	8.183
BF_3	5.337	PBr_3	1.856	butadiene	3.239	DMF	3.520
SO_3	1.618	S_2	0.435	H_2S	4.940	$C_6H_5NH_2$	3.131
Cl_2	1.711	$C_6H_5NO_2$	2.180	C_2H_2	5.532	$CH_3CH=C(CH_3)_2$	4.130
H_2	11.664	PCl_3	2.232	$HCONH_2$	3.409	CH_3F	6.671
SO_2	1.405	N_2O	3.502	styrene	3.006	H_2O	6.126
N_2	4.913	acrylonitrile	3.562	CH_3COCH_3	3.040	$(CH_3)_3As$	4.309
Br_2	1.445	CS_2	2.726	PH_3	5.412	$(CH_3)_3P$	4.566
O_2	0.893	CO_2	4.591	C_6H_6	3.828	$(CH_3)_2S$	4.076
CO	4.606	HF	6.500	toluene	3.719	NH_3	6.996
BCl_3	3.369	HCl	5.486	propylene	4.387	CH_4	11.090
CS	2.981	CH_3CN	5.405	C_6H_5OH	3.179	$C(CH_3)_4$	8.519
HNO_3	3.255	CH_2O	3.008	C_6H_5SH	3.690	$(CH_3)_2O$	5.701
CH_3NO_2	2.441	HCO_2CH_3	3.510	CH_3Cl	4.430	$(CH_3)_3N$	5.931
PF_3	3.388	CH_3CHO	3.042	p-xylene	3.620	-	-
HCN	5.581	C_2H_4	4.529	1,2,5-trimethylbenzene	3.593	-	-

Supp. Table S7. Calculated chemical hardness values of mentioned molecules at B3LYP/SDD level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	2.568	BBr_3	2.812	C_5H_5N	2.906	cyclohexene	5.776
BF_3	5.616	PBr_3	2.026	butadiene	2.712	DMF	3.474
SO_3	2.262	S_2	0.438	H_2S	3.966	$C_6H_5NH_2$	2.692
Cl_2	1.788	$C_6H_5NO_2$	2.345	C_2H_2	4.364	$CH_3CH=C(CH_3)_2$	3.541
H_2	7.409	PCl_3	2.480	$HCONH_2$	3.574	CH_3F	5.482
SO_2	1.951	N_2O	3.892	styrene	2.533	H_2O	4.903
N_2	4.985	acrylonitrile	3.089	CH_3COCH_3	3.049	$(CH_3)_3As$	3.664
Br_2	1.574	CS_2	2.771	PH_3	4.225	$(CH_3)_3P$	3.894
O_2	0.931	CO_2	4.961	C_6H_6	1.214	$(CH_3)_2S$	3.549
CO	5.937	HF	4.778	toluene	3.189	NH_3	4.430
BCl_3	3.380	HCl	4.524	propylene	3.635	CH_4	7.344
CS	2.966	CH_3CN	4.910	C_6H_5OH	3.166	$C(CH_3)_4$	5.657
HNO_3	3.007	CH_2O	2.836	C_6H_5SH	2.819	$(CH_3)_2O$	4.499
CH_3NO_2	2.715	HCO_2CH_3	3.626	CH_3Cl	4.014	$(CH_3)_3N$	4.032
PF_3	4.145	CH_3CHO	2.977	p-xylene	3.068	-	-
HCN	4.986	C_2H_4	3.699	1,2,5-trimethylbenzene	3.089	-	-

Supp. Table S8. Calculated chemical hardness values of mentioned molecules at B3LYP/SDDALL level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	2.473	BBr_3	2.885	C_5H_5N	2.999	cyclohexene	5.569
BF_3	5.784	PBr_3	2.045	butadiene	2.789	DMF	3.577
SO_3	2.168	S_2	0.441	H_2S	3.938	$C_6H_5NH_2$	2.741
Cl_2	1.851	$C_6H_5NO_2$	2.321	C_2H_2	4.524	$CH_3CH=C(CH_3)_2$	3.597
H_2	7.409	PCl_3	2.491	$HCONH_2$	3.708	CH_3F	5.619
SO_2	1.869	N_2O	4.023	styrene	2.601	H_2O	5.037
N_2	5.246	acrylonitrile	3.171	CH_3COCH_3	3.111	$(CH_3)_3As$	3.716
Br_2	1.574	CS_2	2.745	PH_3	4.249	$(CH_3)_3P$	3.827
O_2	1.074	CO_2	5.093	C_6H_6	1.241	$(CH_3)_2S$	3.168
CO	4.598	HF	6.208	toluene	3.278	NH_3	4.325
BCl_3	3.427	HCl	4.544	propylene	3.756	CH_4	7.588
CS	3.066	CH_3CN	4.996	C_6H_5OH	3.053	$C(CH_3)_4$	5.587
HNO_3	3.241	CH_2O	2.993	C_6H_5SH	3.150	$(CH_3)_2O$	4.587
CH_3NO_2	2.799	HCO_2CH_3	3.761	CH_3Cl	3.811	$(CH_3)_3N$	4.046
PF_3	4.026	CH_3CHO	3.091	p-xylene	3.040	-	-
HCN	5.187	C_2H_4	3.842	1,2,5-trimethylbenzene	3.173	-	-

Supp. Table S9. Calculated chemical hardness values of mentioned molecules at MP2/6-31++G(d,p) level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	10.064	BBr_3	6.275	C_5H_5N	5.273	cyclohexene	6.402
BF_3	9.748	PBr_3	5.692	butadiene	4.968	DMF	5.579
SO_3	7.609	S_2	3.765	H_2S	5.786	$C_6H_5NH_2$	4.571
Cl_2	6.313	$C_6H_5NO_2$	5.447	C_2H_2	6.125	$CH_3CH=C(CH_3)_2$	5.045
H_2	9.150	PCl_3	6.352	$HCONH_2$	6.215	CH_3F	7.835
SO_2	6.564	N_2O	7.814	styrene	4.759	H_2O	7.489
N_2	9.801	acrylonitrile	5.821	CH_3COCH_3	6.177	$(CH_3)_3As$	5.053
Br_2	5.388	CS_2	5.605	PH_3	5.802	$(CH_3)_3P$	5.051
O_2	6.624	CO_2	8.175	C_6H_6	5.147	$(CH_3)_2S$	5.160
CO	8.702	HF	9.408	toluene	4.956	NH_3	6.350
BCl_3	6.918	HCl	7.029	propylene	5.446	CH_4	8.017
CS	6.944	CH_3CN	6.652	C_6H_5OH	4.852	$C(CH_3)_4$	6.723
HNO_3	7.308	CH_2O	6.631	C_6H_5SH	4.925	$(CH_3)_2O$	6.349
CH_3NO_2	6.646	HCO_2CH_3	6.936	CH_3Cl	6.471	$(CH_3)_3N$	5.291
PF_3	7.427	CH_3CHO	6.377	p-xylene	4.807	-	-
HCN	7.152	C_2H_4	5.768	1,2,5-trimethylbenzene	4.736	-	-

Supp. Table S10. Calculated chemical hardness values of mentioned molecules at MP2/6-311G level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	6.724	BBr_3	6.242	C_5H_5N	6.232	cyclohexene	7.826
BF_3	11.009	PBr_3	5.071	butadiene	5.838	DMF	6.913
SO_3	6.108	S_2	3.743	H_2S	6.906	$C_6H_5NH_2$	5.766
Cl_2	5.736	$C_6H_5NO_2$	5.351	C_2H_2	7.378	$CH_3CH=C(CH_3)_2$	6.518
H_2	10.423	PCl_3	3.048	$HCONH_2$	7.522	CH_3F	9.392
SO_2	5.311	N_2O	7.665	styrene	5.637	H_2O	8.738
N_2	9.844	acrylonitrile	6.393	CH_3COCH_3	7.487	$(CH_3)_3As$	6.447
Br_2	0.978	CS_2	5.574	PH_3	6.980	$(CH_3)_3P$	6.506
O_2	6.602	CO_2	9.320	C_6H_6	6.342	$(CH_3)_2S$	6.651
CO	9.195	HF	10.540	toluene	6.170	NH_3	7.582
BCl_3	7.109	HCl	7.947	propylene	7.047	CH_4	9.594
CS	6.848	CH_3CN	8.020	C_6H_5OH	6.243	$C(CH_3)_4$	8.069
HNO_3	7.057	CH_2O	7.546	C_6H_5SH	6.197	$(CH_3)_2O$	7.836
CH_3NO_2	6.621	HCO_2CH_3	8.230	CH_3Cl	7.711	$(CH_3)_3N$	6.724
PF_3	7.928	CH_3CHO	7.586	p-xylene	4.382	-	-
HCN	8.693	C_2H_4	7.200	1,2,5-trimethylbenzene	6.034	-	-

Supp. Table S11. Calculated chemical hardness values of mentioned molecules at MP2/LANL2MB level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	5.821	BBr_3	6.824	C_5H_5N	7.051	cyclohexene	12.965
BF_3	11.069	PBr_3	4.814	butadiene	6.883	DMF	7.905
SO_3	4.753	S_2	3.659	H_2S	9.441	$C_6H_5NH_2$	6.838
Cl_2	5.742	$C_6H_5NO_2$	5.692	C_2H_2	9.961	$CH_3CH=C(CH_3)_2$	8.043
H_2	17.328	PCl_3	5.504	$HCONH_2$	8.305	CH_3F	13.591
SO_2	4.290	N_2O	7.045	styrene	6.298	H_2O	13.014
N_2	9.779	acrylonitrile	7.321	CH_3COCH_3	8.210	$(CH_3)_3As$	7.941
Br_2	4.937	CS_2	5.892	PH_3	9.533	$(CH_3)_3P$	8.460
O_2	6.844	CO_2	9.051	C_6H_6	7.294	$(CH_3)_2S$	8.387
CO	9.877	HF	14.058	toluene	7.141	NH_3	13.263
BCl_3	7.539	HCl	10.420	propylene	8.445	CH_4	16.586
CS	7.055	CH_3CN	9.641	C_6H_5OH	6.850	$C(CH_3)_4$	13.471
HNO_3	6.399	CH_2O	8.457	C_6H_5SH	6.985	$(CH_3)_2O$	12.033
CH_3NO_2	6.076	HCO_2CH_3	8.515	CH_3Cl	9.189	$(CH_3)_3N$	11.696
PF_3	7.823	CH_3CHO	8.337	p-xylene	7.001	-	-
HCN	9.893	C_2H_4	8.664	1,2,5-trimethylbenzene	6.959	-	-

Supp. Table S12. Calculated chemical hardness values of mentioned molecules at MP2/SDD level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	6.712	BBr_3	6.183	C_5H_5N	6.075	cyclohexene	9.251
BF_3	10.728	PBr_3	4.913	butadiene	5.668	DMF	7.176
SO_3	6.029	S_2	3.780	H_2S	7.737	$C_6H_5NH_2$	5.598
Cl_2	5.744	$C_6H_5NO_2$	5.177	C_2H_2	7.750	$CH_3CH=C(CH_3)_2$	6.821
H_2	11.620	PCl_3	3.077	$HCONH_2$	7.692	CH_3F	10.180
SO_2	5.247	N_2O	7.434	styrene	5.363	H_2O	9.733
N_2	9.510	acrylonitrile	13.560	CH_3COCH_3	7.495	$(CH_3)_3As$	6.632
Br_2	4.928	CS_2	5.635	PH_3	7.619	$(CH_3)_3P$	7.151
O_2	6.527	CO_2	9.165	C_6H_6	6.171	$(CH_3)_2S$	7.118
CO	8.965	HF	11.458	toluene	6.016	NH_3	8.672
BCl_3	7.182	HCl	8.617	propylene	6.883	CH_4	11.357
CS	6.792	CH_3CN	8.537	C_6H_5OH	5.898	$C(CH_3)_4$	9.254
HNO_3	6.867	CH_2O	7.397	C_6H_5SH	6.079	$(CH_3)_2O$	8.770
CH_3NO_2	6.482	HCO_2CH_3	8.046	CH_3Cl	7.971	$(CH_3)_3N$	7.887
PF_3	8.085	CH_3CHO	7.469	p-xylene	4.306	-	-
HCN	8.559	C_2H_4	6.926	1,2,5-trimethylbenzene	5.904	-	-

Supp. Table S13. Calculated chemical hardness values of mentioned molecules at MP2/SDDALL level in vacuum

Molecule	η	Molecule	η	Molecule	η	Molecule	η
SF_6	6.530	BBr_3	6.213	C_5H_5N	6.232	cyclohexene	9.237
BF_3	10.956	PBr_3	4.878	butadiene	5.819	DMF	7.345
SO_3	5.855	S_2	3.718	H_2S	6.380	$C_6H_5NH_2$	5.736
Cl_2	5.727	$C_6H_5NO_2$	5.220	C_2H_2	8.050	$CH_3CH=C(CH_3)_2$	6.932
H_2	11.620	PCl_3	2.981	$HCONH_2$	7.821	CH_3F	10.394
SO_2	5.076	N_2O	7.642	styrene	5.566	H_2O	9.412
N_2	9.861	acrylonitrile	6.371	CH_3COCH_3	7.472	$(CH_3)_3As$	6.731
Br_2	4.928	CS_2	5.541	PH_3	7.453	$(CH_3)_3P$	6.969
O_2	6.660	CO_2	9.316	C_6H_6	6.340	$(CH_3)_2S$	5.749
CO	9.190	HF	11.473	toluene	5.397	NH_3	8.658
BCl_3	7.037	HCl	7.083	propylene	7.124	CH_4	11.679
CS	6.812	CH_3CN	8.685	C_6H_5OH	6.065	$C(CH_3)_4$	9.213
HNO_3	6.965	CH_2O	7.561	C_6H_5SH	5.831	$(CH_3)_2O$	8.643
CH_3NO_2	6.537	HCO_2CH_3	8.187	CH_3Cl	6.509	$(CH_3)_3N$	7.948
PF_3	7.904	CH_3CHO	7.551	p-xylene	6.032	-	-
HCN	8.903	C_2H_4	7.213	1,2,5-trimethylbenzene	6.054	-	-