Supplementary data for article:

Anđelković, L.; Gruden-Pavlović, M.; Daul, C.; Zlatar, M. The Choice of the Exchange-Correlation Functional for the Determination of the Jahnteller Parameters by the Density Functional Theory. *International Journal of Quantum Chemistry* **2013**, *113* (6), 859–864. https://doi.org/10.1002/qua.24245

SUPPLEMENTARY INFORMATION

TABLE S1 Results of the DFT calculations performed to analyze the JT effect in $C_4H_4^{+\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S2 Results of the DFT calculations performed to analyze the JT effect in $C_5H_5^{\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S3 Results of the DFT calculations performed to analyze the JT effect in $C_6H_6^{+}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S4 Results of the DFT calculations performed to analyze the JT effect in $C_6H_6^{-}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S5 Results of the DFT calculations performed to analyze the JT effect in $C_7H_7^{\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S6 Results of the DFT calculations performed to analyze the JT effect in $CoCp_2$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S7 Results of the DFT calculations performed to analyze the JT effect in Na_3; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S8 Results of the DFT calculations performed to analyze the JT effect in Ag_3; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S9 Results of the DFT calculations performed to analyze the JT effect in $[CuF_6]^{4-}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S10 Results of the DFT calculations performed to analyze the JT effect in $[Mn(acac)_3]$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

TABLE S1 Results of the DFT calculations performed to analyze the JT effect in $C_4H_4^{+\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$C_4H_4^{+\cdot}$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{4h}, {}^2E_g$	-41.0108	-37.5965	-38.3950	-36.0799	-38.5579	-43.9937
$D_{4h}, {}^2B_{2g}$	-40.9128	-37.6039	-38.3915	-36.0702	-38.5682	-44.4491
$D_{4h}, {}^2B_{3g}$	-41.0047	-37.6069	-38.4030	-36.0872	-38.5720	-44.4029
$D_{2h}, {}^2B_{2g}$	-40.9827	-37.6594	-38.4474	-36.1215	-38.6353	-44.5029
$D_{2h}, {}^2B_{3g}$	-41.3045	-37.9131	-38.7073	-36.3968	-38.8712	-44.7313
$E_{JT}, {}^2B_{2g}$	564.1	447.6	450.9	413.8	541.2	433.9
$E_{JT}, {}^2B_{3g}$	2418.2	2469.7	2454.4	2497.1	2413.2	2648.7
Δ	2595.5	2046.2	2096.2	2220.4	1902.7	1842.2
$R_{JT}, {}^2B_{2g}$	0.20	0.20	0.20	0.19	0.21	0.18
$R_{JT}, {}^2B_{3g}$	0.31	0.32	0.32	0.33	0.31	0.32

TABLE S2 Results of the DFT calculations performed to analyze the JT effect in $C_5H_5^{\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$C_5H_5^{\cdot}$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{5h}, {}^2E_1''$	-64.6740	-59.9894	-61.0084	-57.7687	-60.9656	-67.9484
$D_{5h}, {}^2A_2$	-64.6534	-60.0309	-61.0423	-57.7897	-61.0180	-68.3688
$D_{5h}, {}^2B_1$	-64.6534	-60.0311	-61.0423	-57.7898	-61.0181	-68.3689
$C_{2v}, {}^2A_2$	-64.8077	-60.1923	-61.2028	-57.9513	-61.1792	-68.5778
$C_{2v}, {}^2B_1$	-64.8077	-60.1924	-61.2050	-57.9514	-61.1794	-68.5778
$E_{JT}, {}^2A_2$	1244.5	1301.8	1294.5	1303.4	1300.2	1685.7
$E_{JT}, {}^2B_1$	1244.5	1301.0	1312.3	1303.4	1301.0	1688.1
Δ	0.0	-0.8	-17.7	-0.8	-1.6	0.0
$R_{JT}, {}^2A_2$	0.25	0.26	0.26	0.27	0.26	0.27
$R_{JT}, {}^2B_1$	0.25	0.26	0.26	0.27	0.26	0.27

TABLE S3 Results of the DFT calculations performed to analyze the JT effect in $C_6H_6^+$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$C_6H_6^+$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{6h}, {}^2E_{1g}$	-70.9461	-65.3749	-66.6329	-62.9867	-66.4962	-75.2770
$D_{6h}, {}^2B_{3g}$	-70.9141	-65.3983	-66.6494	-62.9899	-66.5330	-75.6597
$D_{6h}, {}^2B_{2g}$	-70.9122	-65.3918	-66.6437	-62.9861	-66.5247	-75.6574
$D_{2h}, {}^2B_{3g}$	-71.0176	-65.5061	-66.7567	-63.0962	-66.6430	-75.7825
$D_{2h}, {}^2B_{2g}$	-71.0212	-65.5015	-66.7528	-63.0952	-66.6352	-75.7776
$E_{JT}, {}^2B_{3g}$	834.9	869.5	865.4	857.4	887.2	990.5
$E_{JT}, {}^2B_{2g}$	879.2	884.8	880.0	880.0	891.2	969.5
Δ	29.1	-37.1	-31.5	-8.1	-62.9	-39.5
$R_{JT}, {}^2B_{3g}$	0.27	0.27	0.27	0.27	0.28	0.27
$R_{JT}, {}^2B_{2g}$	0.27	0.28	0.28	0.28	0.28	0.28

TABLE S4 Results of the DFT calculations performed to analyze the JT effect in $C_6H_6^-$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$C_6H_6^-$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{6h}, {}^2E_{2u}$	-79.1966	-73.3771	-74.5769	-70.5006	-74.2400	-83.1194
$D_{6h}, {}^2A_u$	-79.1919	-73.4082	-74.6030	-70.5162	-74.2741	-83.2387
$D_{6h}, {}^2B_{1u}$	-79.1936	-73.4051	-74.6000	-70.5137	-74.2709	-83.2358
$D_{2h}, {}^2A_u$	-79.2896	-73.5116	-74.7086	-70.6224	-74.3763	-83.3534
$D_{2h}, {}^2B_{1u}$	-79.2848	-73.5067	-74.7018	-70.6174	-74.3722	-83.3512
$C_{2v}, {}^2A_1$	-79.3391	-73.5179	-74.7207	-70.6520	-74.3842	-83.3576
$D_2, {}^2A$	-79.3333	-73.5116	-74.7142	-70.6467	-74.3763	-83.3521
$E_{JT}, {}^2A_u$	788.0	834.0	851.7	856.6	824.3	925.1
$E_{JT}, {}^2B_{1u}$	735.6	819.5	821.1	836.4	817.0	930.8
Δ	38.7	39.5	54.8	40.3	33.1	17.7
$R_{JT}, {}^2A_u$	0.19	0.19	0.19	0.19	0.19	0.29
$R_{JT}, {}^2B_{1u}$	0.18	0.19	0.19	0.19	0.19	0.29
$E_{PJT/JT}, {}^2A_1$	1187.3	884.8	949.3	1095.3	887.8	959.0
$E_{PJT/JT}, {}^2A$	1126.8	859.0	921.1	1072.7	850.1	938.0
Δ	46.8	50.8	52.4	42.7	63.5	44.4
$R_{PJT/JT}, {}^2A_1$	0.62	0.60	0.62	0.59	0.61	0.60
$R_{PJT/JT}, {}^2A$	0.57	0.52	0.56	0.54	0.58	0.50

TABLE S5 Results of the DFT calculations performed to analyze the JT effect in $C_7H_7^{\cdot}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$C_7H_7^{\cdot}$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{7h}, {}^2E_2''$	-91.8973	-85.1798	-86.6458	-82.1156	-86.3152	-96.5656
$D_{7h}, {}^2A_2$	-91.8968	-85.2217	-86.6825	-82.1481	-86.3613	-96.9477
$D_{7h}, {}^2B_1$	-91.8968	-85.2217	-86.6825	-82.1481	-86.3613	-96.9476
$C_{2v}, {}^2A_2$	-92.0026	-85.3361	-86.7961	-82.2641	-86.4750	-97.0868
$C_{2v}, {}^2B_1$	-92.0026	-85.3361	-86.7961	-82.2641	-86.4750	-97.0868
$E_{JT}, {}^2A_2$	853.3	922.7	916.3	935.6	917.1	1122.7
$E_{JT}, {}^2B_1$	853.3	922.7	916.3	935.6	917.1	1122.7
Δ	0.0	0.0	0.0	0.0	0.0	0.0
$R_{JT}, {}^2A_2$	0.16	0.17	0.17	0.17	0.16	0.18
$R_{JT}, {}^2B_1$	0.16	0.17	0.17	0.17	0.16	0.18

TABLE S6 Results of the DFT calculations performed to analyze the JT effect in $CoCp_2$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$CoCp_2$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{5h}, {}^2E_1''$	-142.2897	-130.6751	-133.0479	-125.0391	-133.3851	-149.6008
$D_{5h}, {}^2A_2$	-142.2611	-130.6904	-133.0614	-125.0583	-133.3808	-150.1402
$D_{5h}, {}^2B_1$	-142.2611	-130.6903	-133.0614	-125.0583	-133.3808	-150.1403
$C_{2v}, {}^2A_2$	-142.3620	-130.7848	-133.1558	-125.1444	-133.4847	-150.2304
$C_{2v}, {}^2B_1$	-142.3620	-130.7848	-133.1556	-125.1445	-133.4849	-150.2307
$E_{JT}, {}^2A_2$	813.8	762.2	761.4	694.4	838.0	727.5
$E_{JT}, {}^2B_1$	813.8	761.4	759.8	695.3	839.6	729.1
Δ	0	0	1.6	-0.8	-1.6	-2.4
$R_{JT}, {}^2A_2$	0.35	0.34	0.34	0.32	0.35	0.34
$R_{JT}, {}^2B_1$	0.35	0.34	0.34	0.32	0.35	0.34

TABLE S7 Results of the DFT calculations performed to analyze the JT effect in Na_3; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

Na_3	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{3h}, {}^2E_1'$	-1.7874	-1.5401	-1.6717	-1.2787	-1.5469	-1.7572
$D_{3h}, {}^2A_1$	-1.7826	-1.5570	-1.6904	-1.2739	-1.5943	-1.9306
$D_{3h}, {}^2B_2$	-1.7843	-1.5591	-1.6924	-1.2769	-1.5958	-1.9326
$C_{2v}, {}^2A_1$	-1.8606	-1.6385	-1.7661	-1.3632	-1.6626	-2.0233
$C_{2v}, {}^2B_2$	-1.9034	-1.6838	-1.8034	-1.4574	-1.6836	-2.0792
$E_{JT}, {}^2A_1$	629.1	657.3	610.6	720.3	550.9	747.7
$E_{JT}, {}^2B_2$	960.6	1005.8	895.3	1455.8	708.2	1182.4
Δ	345.2	365.4	300.8	759.8	169.4	450.9
$R_{JT}, {}^2A_1$	1.88	2.01	1.88	2.23	1.74	2.07
$R_{JT}, {}^2B_2$	3.92	4.36	3.68	14.27	2.48	5.49

TABLE S8 Results of the DFT calculations performed to analyze the JT effect in Ag_3; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

Ag_3	LDA	BP86	PW91	BLYP	OPBE	B3LYP
$D_{3h}, {}^2E_1'$	-3.7204	-2.8336	-2.9095	-2.4100	-2.1730	-2.9955
$D_{3h}, {}^2A_1$	-3.6741	-2.8034	-2.8764	-2.3550	-2.1773	-3.1572
$D_{3h}, {}^2B_2$	-3.6724	-2.8040	-2.8762	-2.3545	-2.1801	-3.1577
$C_{2v}, {}^2A_1$	-3.7142	-2.8531	-2.9254	-2.4104	-2.2372	-3.2190
$C_{2v}, {}^2B_2$	-3.7349	-2.8890	-2.9592	-2.4742	-2.2800	-3.2679
$E_{JT}, {}^2A_1$	323.4	400.9	395.2	446.8	483.1	498.5
$E_{JT}, {}^2B_2$	504.1	685.6	669.4	965.5	805.8	888.8
Δ	167.0	289.6	272.6	514.6	345.2	394.4
$R_{JT}, {}^2A_1$	1.16	1.54	1.51	1.76	1.90	1.86
$R_{JT}, {}^2B_2$	2.01	3.39	3.19	9.26	4.42	4.97

TABLE S9 Results of the DFT calculations performed to analyze the JT effect in $[CuF_6]^{4-}$; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in $(amu)^{1/2}$Å

$[CuF_6]^{4-}$	LDA	BP86	PW91	BLYP	OPBE	B3LYP
O_h, ^2E_g	-47.6462	-45.1544	-45.3677	-44.1423	-43.2169	-53.3963
O_h, $^2A_{1g}$	-47.5045	-45.0950	-45.3054	-44.0844	-43.1260	-54.3122
O_h, $^2B_{1g}$	-47.4953	-45.0819	-45.2926	-44.0732	-43.1409	-54.3000
D_{4h}, $^2A_{1g}$	-47.6953	-45.2943	-45.5005	-44.2722	-43.3876	-54.5000
D_{4h}, $^2B_{1g}$	-47.7950	-45.4488	-45.6391	-44.4349	-44.2973	-54.6229
E_{JT}, $^2A_{1g}$	1538.9	1607.5	1573.6	1514.7	2110.0	1514.7
E_{JT}, $^2B_{1g}$	2417.3	3467.4	2794.7	2917.3	9327.1	2604.4
Δ	804.1	1246.1	1117.9	1312.3	7337.3	991.3
R_{JT}, $^2A_{1g}$	1.06	1.25	1.25	1.30	1.65	1.19
R_{JT}, $^2B_{1g}$	1.89	2.53	1.93	2.74	14.02	2.26

TABLE S10 Results of the DFT calculations performed to analyze the JT effect in [Mn(acac)$_3$]; energies are given in eV; the JT parameters E_{JT} and Δ are given in cm^{-1} and R_{JT} in (amu)$^{1/2}$Å

[Mn(acac)$_3$]	LDA	BP86	PW91	BLYP	OPBE	B3LYP
D_3, $^2E_1$	-174.8354	-160.9766	-163.5098	-155.1218	-162.9580	-191.0096
D_3, ^2B	-174.7474	-160.9296	-163.4629	-155.0831	-162.8873	-191.5404
D_3, ^2A	-174.7427	-160.9242	-163.4575	-155.0776	-162.8862	-191.5362
C_2, ^2B	-174.9157	-161.0855	-163.6194	-155.2372	-162.9381	-191.7161
C_2, ^2A	-174.9604	-161.1258	-163.6583	-155.2761	-162.9907	-191.7575
E_{JT}, ^2B	1357.4	1257.4	1262.3	1243.0	409.7	1417.1
E_{JT}, ^2A	1755.9	1626.0	1619.6	1601.0	842.9	1784.9
Δ	360.5	325.0	313.8	313.8	424.3	333.9
R_{JT}, ^2B	0.88	0.98	0.99	0.99	1.44	0.98
R_{JT}, ^2A	1.26	1.44	1.37	1.45	2.06	1.29